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HYDROX:

A One-Dimensional Lagrangian Hydrodynamics Code

University of California

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Milton Samuel Shaw
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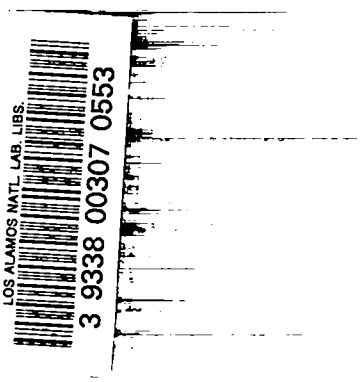

CONTENTS

ABSTRACT 1

I. INTRODUCTION 2

II. HYDRODYNAMIC EQUATIONS OF MOTION 6
- A. Conservation of Mass 6
  - 1. Planar Geometry 7
  - 2. Cylindrical Geometry 7
  - 3. Spherical Geometry 8
- B. Conservation of Momentum 8
  - 1. Planar Geometry 8
  - 2. Cylindrical Geometry 10
  - 3. Spherical Geometry 12
- C. Conservation of Energy 16
  - 1. Planar Geometry 16
  - 2. Cylindrical Geometry 18
  - 3. Spherical Geometry 20
  - 4. The Internal Energy 22
- D. Summary of Equations 23
- E. Finite Difference Equations 25
  - 1. Expansions of a Function on a Lagrangian Lattice 25
  - 2. Space and Time Grid 28
  - 3. Momentum Equation 31
  - 4. Energy Equation 32
  - 5. Kinetic and Internal Energies 34
  - 6. Conservation Properties for the Difference Equations 37

III. INPUT AND OUTPUT 41
- A. Namelist Input for the Input File DATA 42
  - 1. Namelist INP 43
  - 2. Namelist SU 45
  - 3. Namelist ESC 47
  - 4. Namelist BURN 50
- B. Output Files 52
  - 1. DOUT 52
  - 2. XOUT 56
  - 3. OUTPUT 58
  - 4. GASSIN 60
  - 5. DUMPO 62
- C. Graphics 63

IV. HYDROX DESCRIPTION BY SUBROUTINES 66
- A. Summary Descriptions of the Subroutines 66
- B. Chart of the Relation Between Subroutines 74
- C. Variables in Common Blocks Not Already Described 75
- D. Annotated Subroutine Listings and Detailed Notes 79
  - 1. HYDROX-MAIN 79
  - 2. SETUP 84
  - 3. SSU 91
  - 4. ESSU 93
  - 5. BRSU 96
  - 6. CLR 98

7. RSTORE 101
8. EOSDSK 104
9. RHOM 106
10. RBLDUP 109
11. RPOLY 111
12. RSESAME 113
13. JMNMX 115
14. HEI 117
15. GASLM 119
16. BLDSM 123
17. PRNT 126
18. ESUM 129
19. WDUMP 132
20. RDUMP 135
21. OUTGAS 138
22. ICONV 143
23. DIFEQ 146
24. HYDRO 148
25. SINX 154
26. EOS 157
27. PTEOS 160
28. HOM 162
29. USUP 164
30. GAS 169
31. SSBGAS 173
32. MIX 176
33. LFB 183
34. BEQST 187
35. BLDUP 192
36. SPEOS 196
37. POLY 199
38. VISC 202
39. BURN 204
40. ARH 206
41. CJ 208
42. SSB 211
43. FOREST 215
44. FFT 221
45. FFI 223
46. GLTW 224
47. BNDR1 230
48. SL 234
49. SPLTCHK 237
50. SHFT 239
51. SPLIT 241
52. EPP 244
53. DELT 249
54. C 253
55. CUSUP 255
56. CBLDUP 259
57. CPOLY 262
58. CSES 265
59. RLEOS 267
60. RL 269
61. G 274
62. PH 276

E. SESAME Equation-of-State Subroutines 280
1. MATCHK 281
2. TABFCH 282
3. INBUFR 284
4. DPACK 285
5. ISRCHK 286
6. T4INTP 287
7. GETINV 291
8. RATFN1 293
9. T4DATI 295
10. T4RTPE 298
11. INV301 300
12. T4EOSA 302
13. PERTCB 304

V. SAMPLE PROBLEMS 306
A. 1 mm Al Impacting 9404 Using the Forest Fire Model 306
B. 0.5 mm Al Impacting 9404 Using the Forest Fire Model 309
C. 3 cm 9404 in the Buildup Model Pushing 1 cm of Al 311
D. 5 cm Comp. B in the C-J Volume Burn Model Pushing 1 cm of Al with a SESAME Equation of State 313

VI. HMLB AND SESAME EQUATION-OF-STATE LIBRARIES 315
A. HMLB 315
1. Materials in the HMLB HOM EOS Library 316
2. Cross-Reference Table Between HYDROX Variables and SIN Variables for HMLB 316
3. Listing of the EOS Constants in HMLB 319
B. Using the SESAME Option in HYDROX 348
1. Initial State Calculation 348
2. Density and Energy Scaling 348
3. Foams and Phase Transitions 349
4. Interpolation Option 351
5. Table of SESAME Materials in SES2L 351

HYDROX: A ONE-DIMENSIONAL LAGRANGIAN HYDRODYNAMICS CODE*

by

Milton Samuel Shaw and Galen K. Straub

ABSTRACT

HYDROX is a one-dimensional Lagrangian hydrodynamics computer code written in FORTRAN for the solution of problems with plane, cylindrical, or spherical symmetry. A user may request automatic problem zoning, rezoning, and automatic time step controls. Equation-of-state libraries for HOM and SESAME are available. Input to HYDROX is by way of NAMELIST and output may be sent to several different disk files, including a file that is directly readable by the interactive graphics code GAS. A restart capability is also provided. This document is intended to serve as more than just a manual for problem setup; information has been included on the derivation of and differencing schemes for the equation of motion, detailed notes on each subroutine, sample problems, and HMLB and SESAME equation-of-state libraries.

*Los Alamos National Laboratory Identification No. LP-3052.

I. INTRODUCTION

HYDROX is a one-dimensional Lagrangian hydrodynamics computer code written in FORTRAN for the solution of problems with plane, cylindrical, or spherical symmetry. The code may be compiled with up to 20,000 spatial cells on the CDC 7600 series computers and a potentially higher number on the CRAY-1. Versions of the code are available on both the above-mentioned machines as well as the VAX-11.*

HYDROX draws heavily upon the features incorporated in the SIN hydrodynamics code,[1] but also includes several automatic features that simplify user interaction. The user may request the following options: automatic problem zoning, rezoning, and automatic time step controls. HYDROX has been written to reference equation-of-state (EOS) libraries for certain EOS types: HOM,[1] the Barnes EOS form,[2] SESAME tables,[3] and reactive equations of state using HOM. Eight-parameter polynomial EOS's are also available to the user.

The features of SIN for treating explosives were directly adapted into HYDROX. These include Arrhenius reaction kinetics, C-J volume burn with buildup, and Forest Fire.[4-7] Material descriptions for plasticity and spallation are also included.

Input to HYDROX is by way of NAMELIST and output is sent to several different disk files. In addition to printer listable files, HYDROX writes a random access data dump file that is directly readable by the interactive computer graphics code GAS.[8] This file may also be read for cell quantity data and additional information processing. Other dump files may also be written for problem restarting.

HYDROX was written to serve the dual purpose of being the core of a production code for engineering design problems and also a research code

*Execution times for the VAX-11 are about seven times slower than the CDC 7600 for single precision (32-bit) arithmetic and ten times slower for double-precision (64-bit) arithmetic.

for the study and modeling of dynamic flow problems. By using the same code for both types of problems, improved physical descriptions that are being developed are most readily available for design studies. For this reason, we have allowed the user to select options such as extremely small spatial zones or time steps to minimize any numerical error in describing the physics of the dynamic flow. When a highly accurate numerical solution is not needed for a particular portion of a calculation, the user may choose a faster option.

The remainder of the introduction contains a table of consistent sets of units for HYDROX and some useful conversion factors. Section II of this manual discusses the equations of motion in plane, cylindrical, and spherical geometries as well as the accuracy of the finite difference equations. Section III contains input and output information. Section IV is composed of a subroutine-by-subroutine description of the physical models represented in the code and a listing of each subroutine annotated for ease of understanding. Section V contains a short selection of sample problems that illustrate procedures for problem setup and output. Section VI discusses the use of the equation-of-state library HMLB for use with the HOM EOS and the SESAME tabular EOS library.

CONSISTENT SETS OF UNITS FOR HYDROX

Time	μs	s	s
Length	cm	cm	meter
Mass	g	g	kg
Density	g/cm^3	g/cm^3	kg/m^3
Energy	10^{12} ergs	erg	joule
Energy density	Mbar cm^3/g	erg/g	joule/kg
Pressure	Mbar	$dyne/cm^2$	$Newton/m^2$

The preferred set of units is in the first column. EOS libraries contain dimensional constants that are consistent only with this set of units. In using any other set of units the user must make sure they are consistent with internal subroutines that also contain dimensional constants.

Useful Conversion Factors

1 kilobar = 10^9 dynes/cm^2

1 megabar = 10^3 kilobars = 10^{12} dynes/cm^2 = g/cm μs^2

Mbar cm^3/g = 10^{12} erg/g

1 gigapascal = 10 kilobars

1 cm/μs = 10 km/s

1 electron volt = 11604.7 K

Avogadro's number = 6.02252 x 10^{23}/mole

Boltzmann's constant = 1.38054 x 10^{-16} erg/K

Planck's constant = $\hbar$ = 1.054494 x 10^{-27} erg s

Atomic mass unit = 1.66043 x 10^{-24} g/amu

Bohr radius a_0 = 0.529167 x 10^{-8} cm

Rydberg = 2.17971 x 10^{-11} erg

1 Rydberg/a_0^3 = 147.103 Mbar

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II. HYDRODYNAMIC EQUATIONS OF MOTION (In collaboration with B. L. Holian)

In this section we try to give an intuitive derivation of the hydrodynamic equations of motion by considering the appropriate volume element and applying the conservation laws of mass, momentum, and energy. The only completely rigorous manner to derive the equations of motion is to consider the full tensor properties of the stress and strain, and then make the appropriate coordinate transformations corresponding to the symmetry of the problem.

To obtain the appropriate partial differential equations we must consider both Eulerian and Lagrangian coordinates. Eulerian coordinates are a spatially fixed coordinate system sometimes called a laboratory frame of reference. Lagrangian coordinates move through space with the body that they describe and may be thought of as labels for mass points. One may easily transform all quantities from Eulerian to Lagrangian coordinates and we usually visualize a mass element in an Eulerian system, calculate the desired quantities, and transform the results to a Lagrangian system. For a hydrodynamics computer code, the most useful form of the equations is a hybrid of Eulerian positions and velocities used to describe Lagrangian mass points.

A. Conservation of Mass

In order to satisfy the law of conservation of mass, we merely require that the mass of a volume element remain constant even though its shape may change. That is

$$\text{Mass} = \rho V = \text{constant}, \tag{1}$$

where ρ and V are the density and volume of the mass element respectively. In the following,

$$\begin{aligned} r &= \text{Lagrangian position}, \\ R &= \text{Eulerian position}. \end{aligned} \tag{2}$$

At time $t = t_0$ we pick the Lagrangian and Eulerian coordinates to be equal, as well as the length of a mass element:

$$r(t_0) = R(t_0) \quad ; \quad \delta r(t_0) = \delta R(t_0) \quad . \tag{3}$$

At some later time t, the density is $\rho(t)$ and

$$r(t) = r(t_0) \quad \text{and} \quad r(t) + \delta r(t) = r(t_0) + \delta r(t_0) \tag{4}$$

are unchanged with time. The Eulerian coordinates become

$$R(t) \neq R(t_0) \quad \text{and} \quad \delta R(t) \neq \delta R(t_0) \quad . \tag{5}$$

1. Planar Geometry

In Fig. 1 we illustrate a mass element with planar symmetry. The volume of this mass is $dV = \delta R\, \Delta y\, \Delta z$* and its incremental mass is

$$\begin{aligned} \Delta m' &= \rho(t)\, \delta R(t)\, \Delta y\, \Delta z \quad \text{(Eulerian)}, \\ &= \rho_0\, \delta r\, \Delta y\, \Delta z = \text{constant} \quad \text{(Lagrangian)}. \end{aligned} \tag{6}$$

Defining the mass per unit area as $\Delta m = \dfrac{\Delta m'}{\Delta y\, \Delta z}$ and going to the infinitesimal limit, we have

$$dm = \rho\, dR = \rho_0\, dr \quad , \tag{7}$$

where dm is also a mass per unit area.

2. Cylindrical Geometry

In cylindrical coordinates the mass elements may be written:

$$\begin{aligned} dm' &= \rho_0\, r\, dr\, d\theta\, dz \quad \text{(Lagrangian)}, \\ &= \rho(t)\, R\, dR\, d\theta\, dz \quad \text{(Eulerian)}. \end{aligned} \tag{8}$$

*δR and δr are used to denote finite distances for the volume elements, while dR and dr denote infinitesimals. Although not strictly correct, δR and δr may be interchanged with dR and dr by taking a limit where δR and δr go to zero.

We can define a mass per unit length dm = dm'/dz and, assuming cylindrical symmetry for the problem, integrate over θ to get

$$dm = 2\pi\rho_0 \, r \, dr = 2\pi\rho(t) \, R \, dR \quad . \tag{9}$$

3. Spherical Geometry

In spherical coordinates the mass elements may be written

$$\begin{aligned} dm = dm' &= \rho_0 \, r^2 \, dr \sin\theta \, d\theta \, d\phi \quad \text{(Lagrangian)}, \\ &= \rho(t) \, R^2 \, dR \sin\theta \, d\theta \, d\phi \quad \text{(Eulerian)}. \end{aligned} \tag{10}$$

Integration over θ and φ gives

$$dm = 4\pi\rho_0 \, r^2 \, dr = 4\pi\rho(t) \, R^2 \, dR \quad . \tag{11}$$

B. Conservation of Momentum

To determine the net momentum flux through a mass element at any time, we use Newton's equation of motion in the form:

$$\frac{\text{force in the R direction}}{\text{unit mass}} = \frac{F_R}{dm} = \frac{\partial u_R}{\partial t} \equiv \dot{u}_R \quad , \tag{12}$$

where u_R = velocity in the R direction.

1. Planar Geometry

Figure 1 shows a planar mass element subjected to a stress σ_r in the positive direction and a stress $\sigma_r + \Delta\sigma_r$ in the negative direction. Since stress is defined as the force per unit area, then

$$F_R = \sigma_r \, \Delta y \, \Delta z \quad . \tag{13}$$

The net force acting on the volume element is $F_R - F_{R+\delta R}$, giving

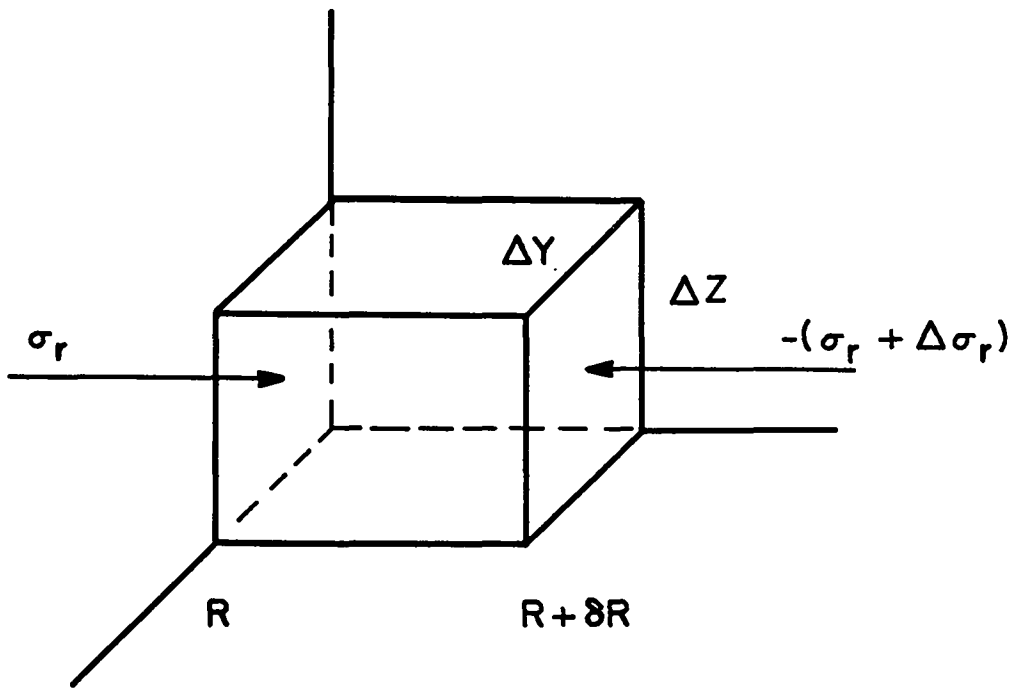


Fig. 1.
A planar mass element subjected to a stress σ_r in the positive direction and a stress $\sigma_r + \Delta\sigma_r$ in the negative direction. The cross-sectional area that these stresses act upon is $\Delta y\ \Delta z$.

$$\frac{\partial u_R}{\partial t} = \frac{F_R - F_{R+\delta R}}{dm'} = \frac{\sigma_r \Delta_y \Delta_z}{\rho\, \delta R\, \Delta y\, \Delta z} - \frac{(\sigma_r + \Delta\sigma_r)\Delta y\, \Delta z}{\rho\, \delta R\, \Delta y\, \Delta z}$$

$$= -\frac{1}{\rho}\frac{\Delta\sigma_r}{\delta R} \xrightarrow[\lim\, \delta R \to 0]{} -\frac{1}{\rho}\frac{\partial \sigma_r}{\partial R} \quad , \tag{14}$$

or

$$\frac{\partial u_R}{\partial t} = -\frac{1}{\rho}\frac{\partial \sigma_R}{\partial R} \quad . \tag{15}$$

Transforming to the Lagrangian variables $dm = \rho_0\, dr$ by using the relation $\rho_0\, dr = \rho\, dR$, we have

$$\left(\frac{\partial u}{\partial t}\right)_r = -\frac{1}{\rho_0}\left(\frac{\partial \sigma}{\partial r}\right)_t = -\left(\frac{\partial \sigma}{\partial m}\right)_t \quad , \tag{16}$$

where $(\partial u/\partial t)_r$ denotes the acceleration of a single Lagrangian mass point with coordinate r and the stress gradient is evaluated at constant time t.

2. Cylindrical Geometry

For a system with cylindrical symmetry, we must include the contributions to the stress from the θ-direction as well as the r-direction. Figure 2 shows a mass element in cylindrical coordinates subjected to the stresses σ_{rr} and $\sigma_{rr} + \Delta\sigma_{rr}$ in the radial direction, and stresses $+\sigma_{\theta\theta}$ and $-\sigma_{\theta\theta}$ in the angular direction. We need only worry about the components of $\sigma_{\theta\theta}$ in the radial direction because the net force in the θ-direction at the center of the mass point is

$$F_\theta = +\sigma_{\theta\theta} \cos\frac{\theta}{2}\, \delta R\, \Delta z - \sigma_{\theta\theta} \cos\frac{\theta}{2}\, \delta R\, \Delta z = 0 \quad . \tag{17}$$

In the radial direction we have

$$F_R = m\dot{u}_R = \rho R\, \delta R\, \Delta\theta\, \Delta z\, \dot{u}_R$$

$$= \sigma_{rr} R \sin\Delta\theta\, \Delta z - (\sigma_{rr} + \Delta\sigma_{rr})(R + \delta R) \sin\Delta\theta\, \Delta z + 2\sigma_{\theta\theta} \sin\frac{\Delta\theta}{2}\, \delta R\, \Delta z \tag{18}$$

$$= -\sigma_{rr}\, \delta R \sin\Delta\theta\, \Delta z - \Delta\sigma_{rr}(R + \delta R) \sin\Delta\theta\, \Delta z + 2\sigma_{\theta\theta} \sin\frac{\Delta\theta}{2}\, \delta R \Delta z \quad .$$

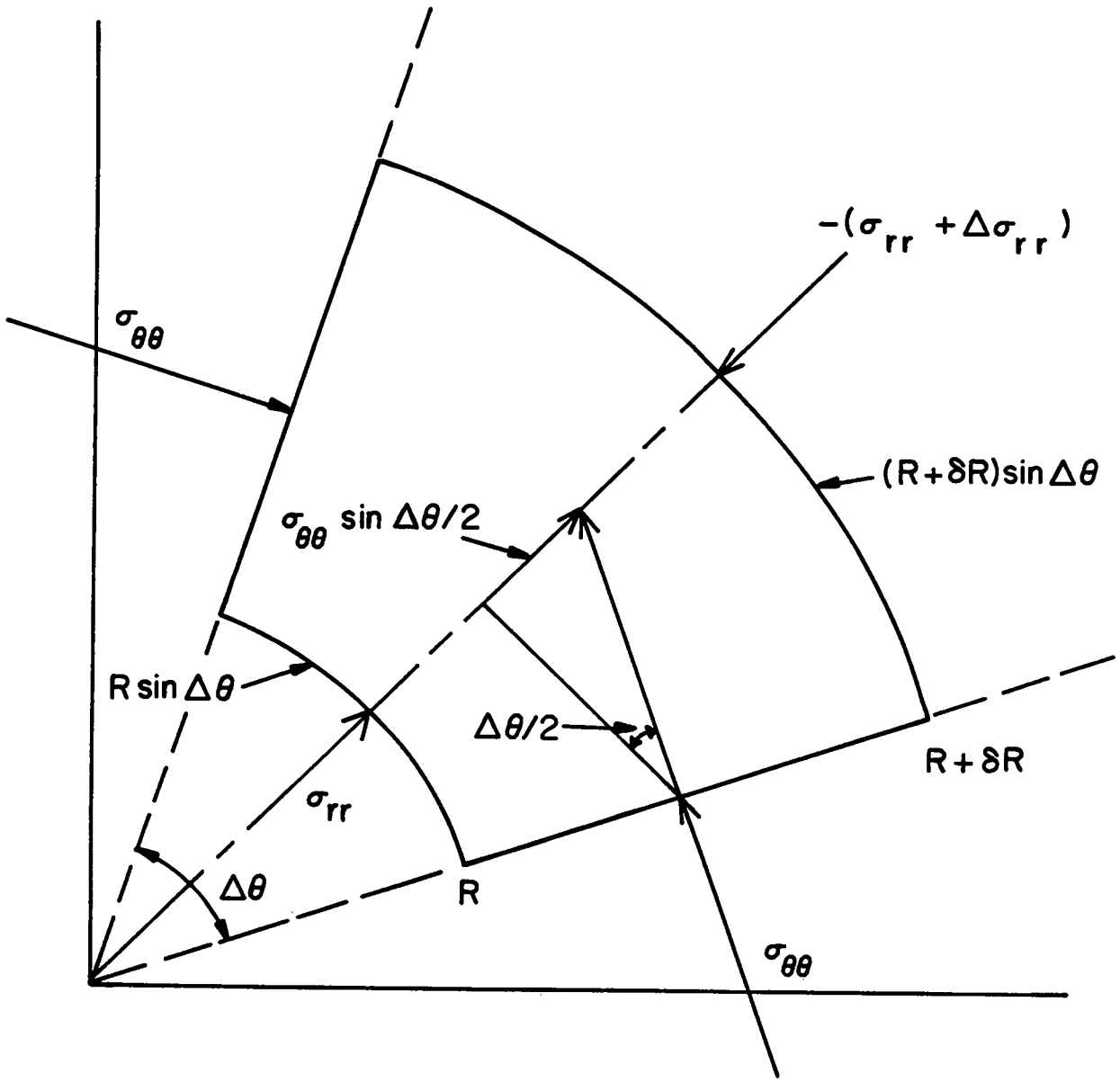


Fig. 2.
A mass element in cylindrical coordinates subjected to the stresses σ_{rr} and $-(\sigma_{rr} + \Delta\sigma_{rr})$ in the radial direction and to $+\sigma_{\theta\theta}$ and $-\sigma_{\theta\theta}$ in the angular direction.

Because mass = $\rho R\ \delta R\ \Delta\theta\ \Delta z$, we have

$$\rho\dot{u}_R = -\frac{\sigma_{rr}}{R}\frac{\sin\Delta\theta}{\Delta\theta} - \frac{\Delta\sigma_{rr}}{\delta R}\left(1+\frac{\delta R}{R}\right)\frac{\sin\Delta\theta}{\Delta\theta} + \frac{2\sigma_{\theta\theta}}{R}\frac{\sin\Delta\theta/2}{\Delta\theta} \quad .$$

In the limit as δR, $\Delta\theta$ goes to zero, $\frac{\sin\Delta\theta}{\Delta\theta} \to 1$ giving

$$\rho\dot{u}_R = -\frac{\sigma_{rr}}{R} - \frac{\partial\sigma_{rr}}{\partial R} + \frac{\sigma_{\theta\theta}}{R} + O(\delta R) + O(\Delta\theta) \quad ,$$

where $O(x) \equiv$ order of x.

Thus,

$$\rho\dot{u}_R = -\frac{\partial\sigma_{rr}}{\partial R} + \frac{\sigma_{\theta\theta} - \sigma_{rr}}{R} \quad . \tag{19}$$

To change to Lagrangian coordinates, we use $dm = \rho_0\ r\ dr = \rho R\ dR \Rightarrow dr = dm/\rho R$, giving

$$\left(\frac{\partial u_R}{\partial t}\right)_r = -R\left(\frac{\partial\sigma_{rr}}{\partial m}\right)_t + \frac{(\sigma_{\theta\theta} - \sigma_{rr})}{\rho R} \quad , \tag{20}$$

where $(\ )_r$ denotes that we are considering a single Lagrangian mass element (constant r or dm), and the u_R is the velocity measured in the Eulerian reference frame.

3. Spherical Geometry

A spherical volume element is shown in Fig. 3. The spherical case is slightly more difficult to visualize because $\Delta\phi$ is measured in the x-y plane and the arc length swept by a rotation in ϕ must be projected up to the volume element. We have introduced the quantity $\Delta\phi'$ (not equal to $\Delta\phi$) to help avoid confusion. As in the cylindrical case, there are components in the radial directions from $\sigma_{\theta\theta}$ and $\sigma_{\phi\phi}$, but no net force in either the θ or ϕ direction.

(a)

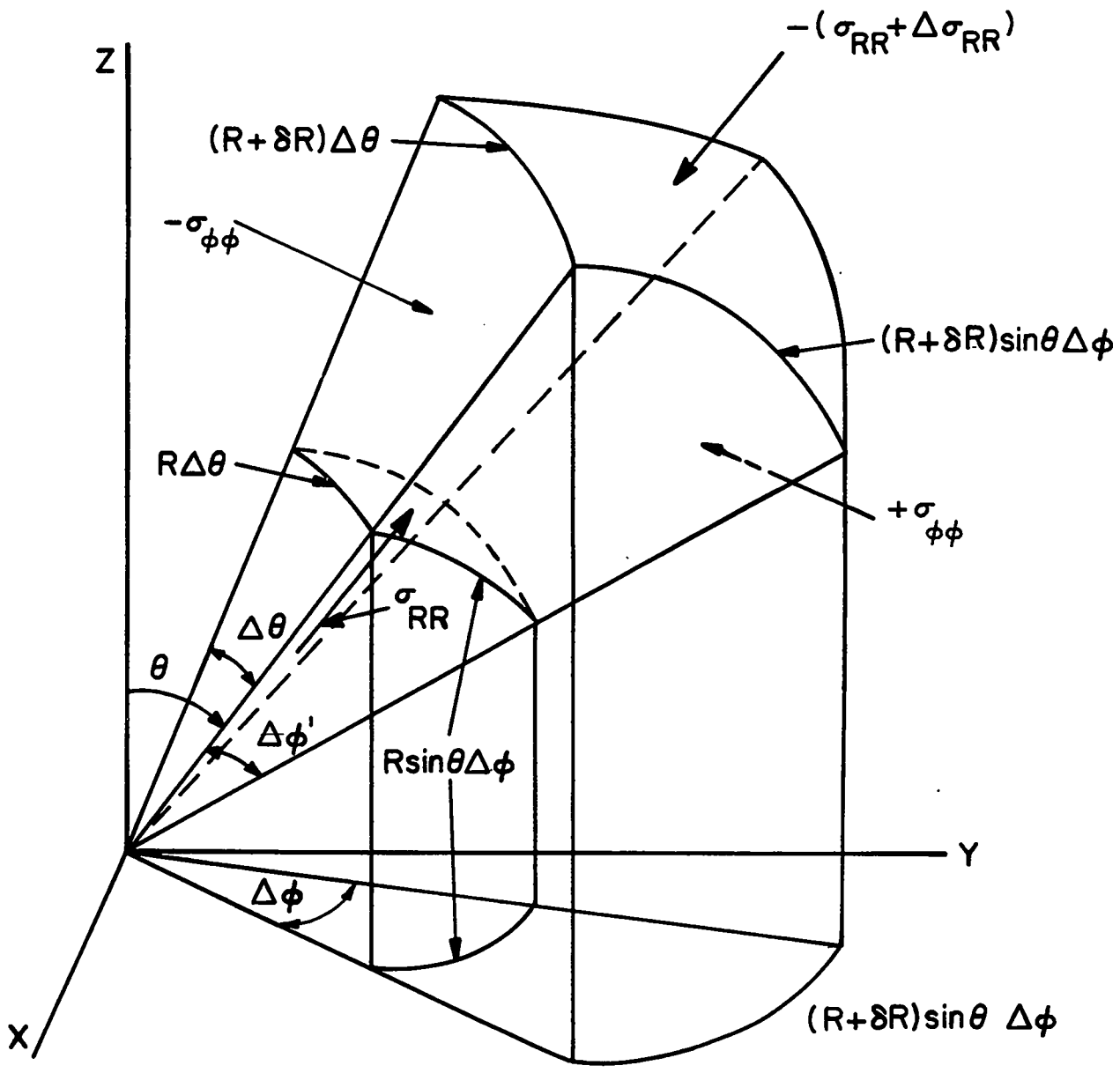


Fig. 3a.
A spherical volume element subjected to the stresses σ_{RR} and $-(\sigma_{RR} + \Delta\sigma_{RR})$ in the radial direction, $+\sigma_{\theta\theta}$ and $-\sigma_{\theta\theta}$ in one angular direction, and $+\sigma_{\phi\phi}$ and $-\sigma_{\phi\phi}$ in the other angular direction. Note that $\Delta\phi \neq \Delta\phi'$.

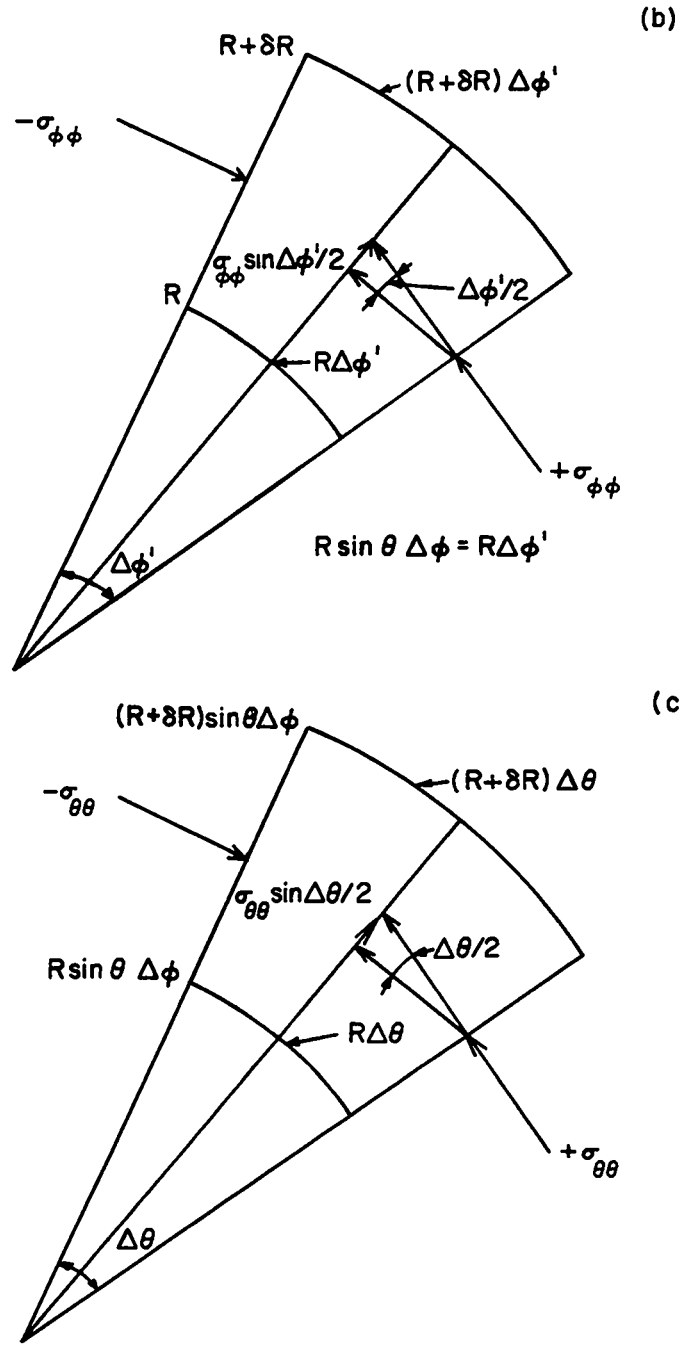


Fig. 3b,c.

(b) The stress $+\sigma_{\phi\phi}$ and $-\sigma_{\phi\phi}$ acting on the spherical volume element depend on the angle $\Delta\phi'$ and not on its projection in the x-y plane, $\Delta\phi$.

(c) For the θ-direction, the stresses $+\sigma_{\theta\theta}$ and $-\sigma_{\theta\theta}$ are dependent only upon $\Delta\theta$.

Consider first the stresses $\sigma_{\phi\phi}$ acting on the volume element as shown in Fig. 3b. The net force in the radial direction from the stresses acting on each side of the volume element is

$$\left(\sigma_{\phi\phi} \sin \frac{\Delta\phi'}{2} + \sigma_{\phi\phi} \sin \frac{\Delta\phi'}{2}\right) R\ \delta R\ \Delta\theta = 2\sigma_{\phi\phi} \sin \frac{\Delta\phi'}{2} R\ \delta R\ \Delta\theta \quad , \tag{21}$$

with $\sigma_{\phi\phi}$ acting on an area $R\ \delta R\ \Delta\theta$. By requiring the arc length swept by the $\Delta\phi$ rotation to be the same as the $\Delta\phi'$ rotation, we have

$$\begin{aligned} R\Delta\phi' &= R \sin\theta\ \Delta\phi \quad , \\ \Delta\phi' &= \sin\theta\ \Delta\phi \quad , \end{aligned} \tag{22}$$

or making Eq. (21)

$$2\sigma_{\phi\phi} \sin[\tfrac{1}{2} \sin\theta\ \Delta\phi]\, R\, \delta R\ \Delta\theta \quad . \tag{23}$$

The net force in the radial direction from the $\sigma_{\theta\theta}$'s is

$$2\sigma_{\theta\theta} \sin \frac{\Delta\theta}{2} R\ \delta R \sin\theta\ \Delta\phi \quad . \tag{24}$$

The net total force in the radial direction is

$$\begin{aligned} F_R = {} & \sigma_{rr} R^2 \sin\theta\ \Delta\theta\ \Delta\phi - (\sigma_{rr} + \Delta\sigma_{rr})(R + \delta R)^2 \sin\theta\ \Delta\theta\ \Delta\phi \\ & + 2\sigma_{\phi\phi} \sin[\tfrac{1}{2} \sin\theta\ \Delta\phi]\, R\, \delta R\ \Delta\theta + 2\sigma_{\theta\theta} \sin \frac{\Delta\theta}{2} R\ \delta R \sin\theta\ \Delta\phi \quad . \end{aligned} \tag{25}$$

$$\frac{F_R}{\text{unit mass}} = \frac{F_R}{\rho R^2 \sin\theta\ \Delta\theta\ \Delta\phi} \Rightarrow \rho \frac{\partial U_R}{\partial t} = \frac{F_R}{R^2\ \delta R \sin\theta\ \Delta\theta\ \Delta\phi} \quad .$$

In Eq. (25) we again take the limit of small $\Delta\theta$ and $\Delta\phi$:

$$\begin{aligned} \sin \frac{\Delta\theta}{2} &\to \frac{\Delta\theta}{2} \quad , \\ \sin[\tfrac{1}{2} \sin\theta\ \Delta\phi] &\to \tfrac{1}{2} \sin\theta\ \Delta\phi \quad . \end{aligned}$$

Thus,

$$\rho \frac{\partial u_R}{\partial t} = -\sigma_{rr}\left(\frac{2}{R} + \frac{\delta R}{R^2}\right) - \frac{\Delta\sigma_{rr}}{\delta R}\left(1 + \frac{2\delta R}{R} + \frac{(\delta R)^2}{R^2}\right) + \frac{\sigma_{\phi\phi}}{R} + \frac{\sigma_{\theta\theta}}{R} \quad ,$$

or, taking the limit as δR goes to zero,

$$\rho \frac{\partial u_R}{\partial t} = -\frac{\partial \sigma_{rr}}{\partial R} + \frac{1}{R}(\sigma_{\phi\phi} + \sigma_{\theta\theta} - 2\sigma_{rr}) + O(\delta R) + O(\delta R^2) \quad .$$

Because of the spherical symmetry, $\sigma_{\phi\phi} = \sigma_{\theta\theta}$, and if we neglect terms of order δR and higher, our result is

$$\rho \frac{\partial u_R}{\partial t} = -\frac{\partial \sigma_{rr}}{\partial R} - \frac{2}{R}(\sigma_{rr} - \sigma_{\theta\theta}) \quad . \tag{26}$$

To go to Lagrangian coordinates we use $dm = \rho R^2\, dR$, and obtain the acceleration equation for the mass point labeled with the coordinate r:

$$\left(\frac{\partial u_R}{\partial t}\right)_r = -R^2\left(\frac{\partial \sigma_{rr}}{\partial m}\right)_t + \frac{2(\sigma_{\theta\theta} - \sigma_{rr})}{\rho R} \quad . \tag{27}$$

C. Conservation of Energy

We wish to calculate the increase in the <u>total</u> energy of a mass element during some time Δt due to the work done by the stresses in the radial direction. The stresses in the angular direction do <u>no</u> work on the mass element because there is no motion in the angular directions.

1. Planar Geometry

A planar mass element is depicted in Fig. 4 at times t and $t + \Delta t$. Letting ΔE be the change in energy per unit mass = $\rho \delta R\, \Delta y\, \Delta z$, we can write (energy = force x distance):

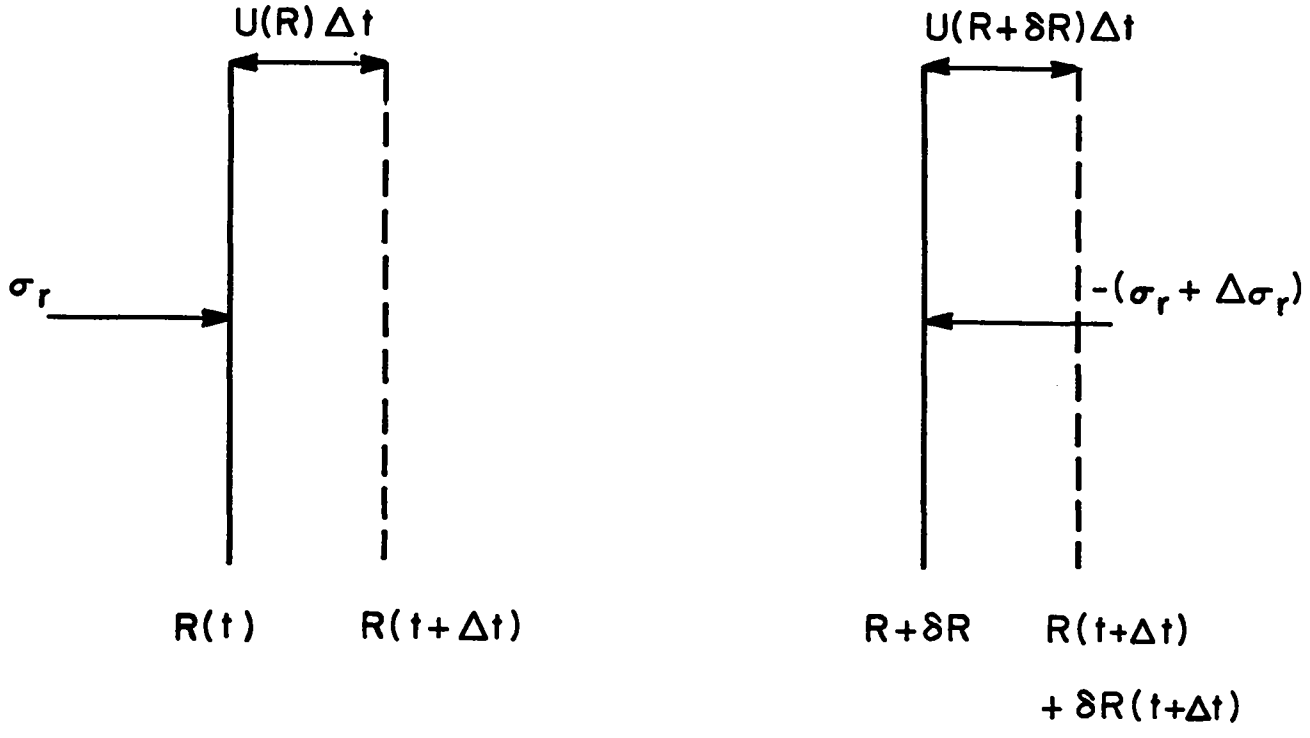


Fig. 4.
A planar mass element at time t (solid line) and t + Δt (dashed line).

$$\Delta E = \frac{\sigma_r \, \Delta y \, \Delta z \, u(R) \, \Delta t - (\sigma_r + \Delta\sigma_r)\Delta y \, \Delta z \, u(R + \delta R)\Delta t}{\rho \delta R \, \Delta y \, \Delta z} \quad ,$$

$$\rho \frac{\partial E}{\partial t} = \frac{\sigma_r u(R) - (\sigma_r + \Delta\sigma_r)u(R + \delta R)}{\delta R} \quad . \tag{28}$$

We may expand $u(R + \delta R)$ about R:

$$u(R + \delta R) = u(R) + \left(\frac{\partial u}{\partial R}\right)\delta R + \cdots \quad .$$

Substituting this result to first order in δR into Eq. (28), we get

$$\rho\left(\frac{\partial E}{\partial t}\right) = - \frac{\Delta\sigma_r u}{\delta R} - \sigma_r\left(\frac{\partial u}{\partial R}\right) - \Delta\sigma_r\left(\frac{\partial u}{\partial R}\right) \quad . \tag{29}$$

Taking the limit as $\delta R \to 0$,

$$\rho\left(\frac{\partial E}{\partial t}\right) = - u\left(\frac{\partial \sigma_r}{\partial R}\right) - \sigma_r\left(\frac{\partial u}{\partial R}\right) \quad .$$

In the limit $\delta R \to 0$, then $\Delta\sigma_r \to 0$.

Using $dm = \rho \, dR$, we can write

$$\left(\frac{\partial E}{\partial t}\right)_r = - \frac{\partial}{\partial m}(\sigma_r u) \quad , \tag{30}$$

where the $(\,)_r$ expresses the fact that we are considering a single Lagrangian mass element.

2. Cylindrical Geometry

The calculation for cylindrical geometry proceeds in the same manner as the planar case except that the unit mass element = $\rho R \delta R \, \Delta\theta \, \Delta z$. The angular stresses $\sigma_{\theta\theta}$ and the axial stresses σ_{zz} do no work because motion is permitted in the R direction only. Figure 5 shows the appropriate mass element at times t and $t + \Delta t$.

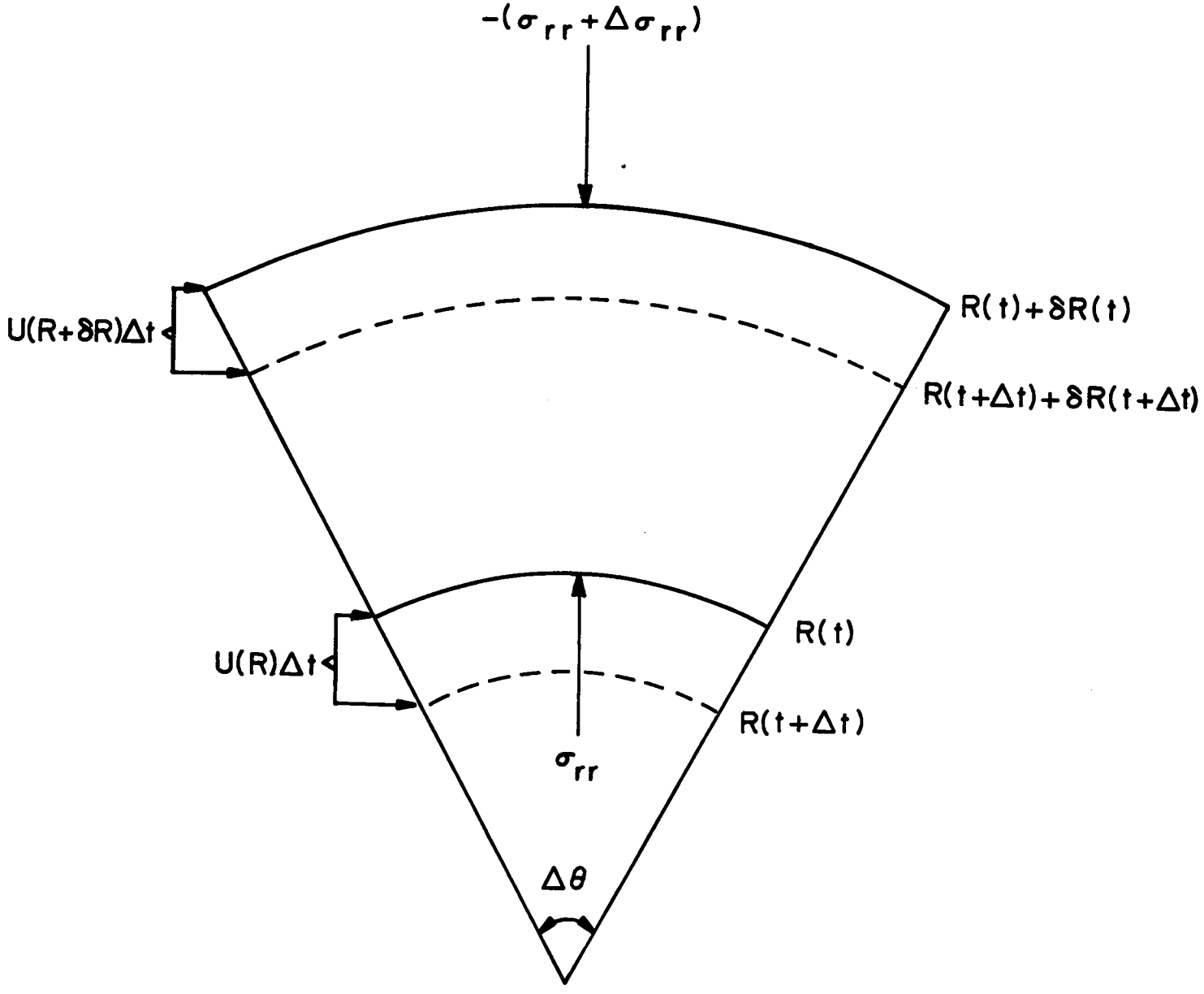


Fig. 5.
A cylindrical mass element at times t (solid lines) and t + Δt (dashed lines). The angular stresses, $+\sigma_{\theta\theta}$ and $-\sigma_{\theta\theta}$, do no work because motion is permitted in the radial direction only.

The change in energy per unit mass is again calculated by considering the distance the forces acting on the mass element move.

$$dE = \frac{+\sigma_{rr}R(t)\,\Delta\theta\;\Delta z[u(R)\Delta t] \;-\; (\sigma_{rr}+\Delta\sigma_{rr})(R+\delta R)\Delta\theta\;\Delta z[u(R+\delta R)\Delta t]}{\rho R\;\delta R\;\Delta\theta\;\Delta z} \quad .$$

$$\frac{\partial E}{\partial t} = +\frac{\sigma_{rr}u(R)}{\rho\delta R} - \frac{(\sigma_{rr}+\Delta\sigma_{rr})(R+\delta R)u(R+\delta R)}{\rho R\;\delta R} \quad .$$

Using $u(R+\delta R) = u(R) + (\partial u/\partial R)\delta R + \cdots$, we obtain

$$\frac{\partial E}{\partial t} = -\left\{\frac{\sigma_{rr}u(R)}{R} + \sigma_{rr}\frac{\partial u}{\partial R} + \sigma_{rr}\left(\frac{\partial u}{\partial R}\right)\frac{\delta R}{R} + \frac{\Delta\sigma_{rr}u(R)}{\delta R} + \frac{\Delta\sigma_{rr}u(R)}{\rho R}\right.$$
$$\left. + \Delta\sigma_{rr}\left(\frac{\partial u}{\partial r}\right) + \Delta\sigma_{rr}\left(\frac{\partial u}{\partial R}\right)\frac{\delta R}{R}\right\} \quad , \tag{31}$$

$$= O(1) + O(1) + O(\delta R) + O(1) + O(\Delta\sigma_{rr}) + O(\Delta\sigma_{rr}) + O(\Delta\sigma_{rr}\delta R) \quad .$$

In the last equation we have written the relative order of the terms for Eq. (31). Keeping only the leading order terms we have, after taking the appropriate limits,

$$\rho\frac{\partial E}{\partial t} = -\left\{\sigma_{rr}\frac{u}{R} + \sigma_{rr}\left(\frac{\partial u}{\partial R}\right) + \left(\frac{\partial\sigma_{rr}}{\partial R}\right)u\right\} \quad .$$

Using $dm = \rho R\,dR$ or $\partial R/\partial m = 1/\rho R$, we write

$$\left(\frac{\partial E}{\partial t}\right)_r = -\frac{\partial}{\partial m}(\sigma_{rr}uR) \quad , \tag{32}$$

for the Lagrangian mass element labeled by r.

3. Spherical Geometry

A spherical mass element is shown in Fig. 6 where a unit mass is $\rho R^2\,\delta R\sin\theta\,\Delta\theta\,\Delta\phi$. In the same manner as for the planar and cylindrical cases, the change in energy per unit mass due to the work done by the radial stresses is

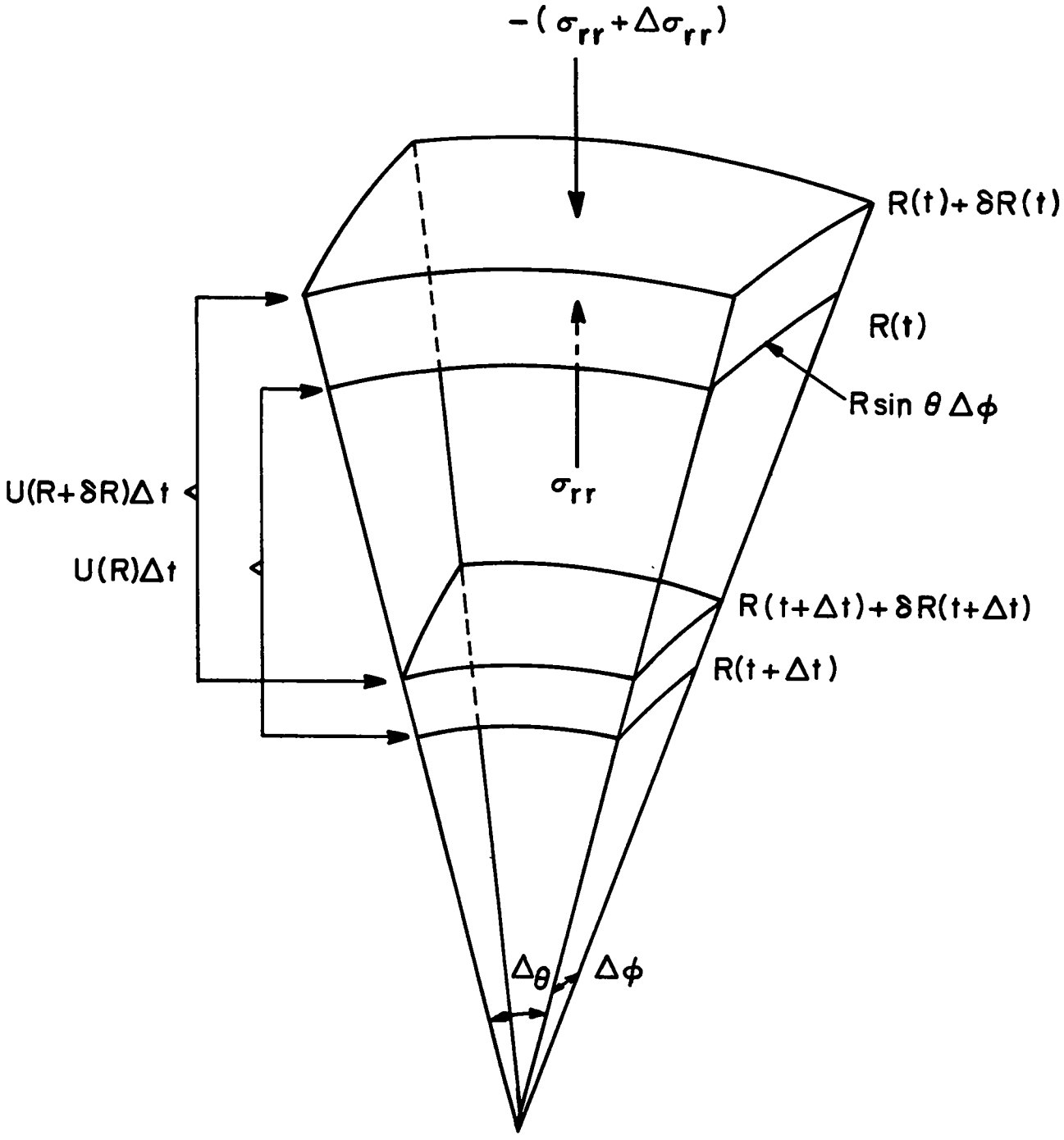


Fig. 6.
A spherical mass element at times t and t + Δt. The two sets of stresses in the angular direction do no net work and are not shown here.

$$dE = \frac{\sigma_{rr}(R\Delta\theta)(R\sin\theta\ \Delta\phi)[u(R)\Delta t] - (\sigma_{rr}+\Delta\sigma_{rr})(R+\delta R)\Delta\theta\,(R+\delta R)\sin\theta\,\Delta\phi[u(R+\delta R)\Delta t]}{\rho R^2\ \delta R\ \sin\theta\ \Delta\theta\ \Delta\phi}$$

or, rewriting, the rate of change of energy is given by

$$\rho\frac{\partial E}{\partial t} = \frac{\sigma_{rr}R^2u(R) - (\sigma_{rr}+\Delta\sigma_{rr})(R+\delta R)^2u(R+\delta R)}{R^2\,\delta R} \quad .$$

Using $u(R+\delta R) = u(R) + (\partial u/\partial R)\delta R + \cdots$, we may obtain

$$\rho\frac{\partial E}{\partial t} = -\left\{\frac{2\sigma_{rr}u}{R} + \frac{\sigma_{rr}\delta Ru}{R^2} + \sigma_{rr}\left[1+\frac{2\delta R}{R}+\left(\frac{\delta R}{R}\right)^2\right]\left(\frac{\partial u}{\partial R}\right) + \frac{\Delta\sigma_{rr}}{\delta R}\left[1+\frac{2\delta R}{R}+\left(\frac{\delta R}{R}\right)^2\right]u\right.$$

$$\left. + \Delta\sigma_{rr}\left[1+\frac{2\delta R}{R}+\left(\frac{\delta R}{R}\right)^2\right]\left(\frac{\partial u}{\partial R}\right)\right\} \quad .$$

Keeping only the leading order terms, our result becomes

$$\rho\frac{\partial E}{\partial t} = -\left\{\frac{2\sigma_{rr}u}{R} + u\left(\frac{\partial\sigma_{rr}}{\partial R}\right) + \sigma_{rr}\left(\frac{\partial u}{\partial R}\right)\right\} \quad .$$

Again, $\sigma_{\theta\theta}$ and $\sigma_{\phi\phi}$ do <u>no</u> work because of the requirement that there be no motion in the θ and ϕ directions. To write in a Lagrangian form, use $dm = \rho R^2\,dR$ to get $1/\rho R = R\,\partial R/\partial m$, and

$$\left(\frac{\partial E}{\partial t}\right)_r = -\frac{\partial}{\partial m}(R^2u\sigma_{rr}) \quad . \tag{33}$$

4. The Internal Energy

For some calculations, it is more convenient to work directly with the internal energy than with the total energy. The internal energy, I, may be determined from

$$E = \frac{1}{2} u^2 + I \quad ,$$

where the first term in this expression gives the kinetic energy. Equations (30), (32), and (33) may be written in the combined form

$$\left(\frac{\partial E}{\partial t}\right)_r = - \frac{\partial}{\partial m}(\sigma_{rr} u R^{d-1}) \quad ,$$

where d = 1, 2, or 3 for planar, cylindrical, or spherical geometry, respectively. We now wish to obtain the time rate of change of the internal energy. Thus,

$$\left(\frac{\partial E}{\partial t}\right) = u\left(\frac{\partial u}{\partial t}\right) + \left(\frac{\partial I}{\partial t}\right)_r = -uR^{d-1}\left(\frac{\partial \sigma_{rr}}{\partial m}\right)_t - \sigma_{rr}\left(\frac{\partial}{\partial m} uR^{d-1}\right)_t \quad .$$

In analogy with the above expression for the conservation of total energy, we may write the conservation of momentum relation as

$$\left(\frac{\partial u}{\partial t}\right)_r = -R^{d-1}\left(\frac{\partial \sigma_{rr}}{\partial m}\right)_t + (d - 1) \frac{(\sigma_{\theta\theta} - \sigma_{rr})}{\rho R} \quad .$$

Using this expression allows one to write

$$\left(\frac{\partial I}{\partial t}\right)_r = -\sigma_{rr}\left(\frac{\partial u R^{d-1}}{\partial m}\right)_t + \frac{u(d - 1)}{\rho R} (\sigma_{rr} - \sigma_{\theta\theta}) \quad .$$

D. Summary of Equations

In this section we shall summarize the equations obtained by the application of the conservation laws of mass, momentum, and energy on a one-dimensional Lagrangian mass element under stress.

Conservation of mass requires

$$\begin{aligned} dm &= \rho dR = \rho_0 dr \quad \text{(planar)}, \\ &= 2\pi\rho R dR = 2\pi\rho_0 r dr \quad \text{(cylindrical)}, \\ &= 4\pi\rho R^2 dR = 4\pi\rho_0 r^2 dr \quad \text{(spherical)}. \end{aligned} \tag{34}$$

Conservation of momentum gives

$$\begin{aligned} \left(\frac{\partial u}{\partial t}\right)_r &= -\frac{1}{\rho_0}\left(\frac{\partial \sigma_r}{\partial r}\right)_t = -\left(\frac{\partial \sigma_r}{\partial m}\right)_t \quad \text{(planar)}, \\ &= -R\left(\frac{\partial \sigma_{rr}}{\partial m}\right)_t + \frac{(\sigma_{\theta\theta} - \sigma_{rr})}{\rho R} \quad \text{(cylindrical)}, \\ &= -R^2\left(\frac{\partial \sigma_{rr}}{\partial m}\right)_t + 2\,\frac{(\sigma_{\theta\theta} - \sigma_{rr})}{\rho R} \quad \text{(spherical)}. \end{aligned} \tag{35}$$

Conservation of energy gives

$$\begin{aligned} \left(\frac{\partial E}{\partial t}\right)_r &= -\frac{\partial}{\partial m}(\sigma_r u) \quad \text{(planar)}, \\ &= -\frac{\partial}{\partial m}(\sigma_r u R) \quad \text{(cylindrical)}, \\ &= -\frac{\partial}{\partial m}(\sigma_r u R^2) \quad \text{(spherical)}. \end{aligned} \tag{36}$$

E. Finite Difference Equations

In the present section we will present the procedure for evaluating the differential equations for fluid motion on a finite Lagrangian space-time grid. We begin with a general discussion of Taylor series expansions of known functions and then use these results for the fluid equations. At the end of this section the conservation properties of the difference equations are discussed. For simplicity we give only the results for planar geometry.

1. Expansions of a Function on a Lagrangian Lattice

Consider some function f(r) of the Lagrangian coordinate r on a grid of Lagrangian points as shown in Fig. 7. The distance between the $j-\frac{1}{2}$ and $j+\frac{1}{2}$ boundaries is called r_j for cell j. The function f(r) evaluated at the center of the cell is written f_j and the same function evaluated at the $j+\frac{1}{2}$ boundary is written $f_{j+\frac{1}{2}}$.

Assume that the values of f(r) are known at the cell center and we want to calculate spatial derivatives of f at cell boundaries; that is, we know f_j, $f_{j\pm1}$, $f_{j\pm2}$, $\cdots$ and we want to calculate $(\partial f/\partial r)_{j+\frac{1}{2}}$. Because $j+\frac{1}{2}$ is the boundary between cell j and cell j+1, we will need to use f_j and f_{j+1} to determine the derivative. To do this, we make a Taylor series expansion of our function about the point $j+\frac{1}{2}$.

$$f_j = f_{j+\frac{1}{2}} - \left(\frac{\partial f}{\partial r}\right)_{j+\frac{1}{2}} \frac{r_j}{2} + \frac{1}{2}\left(\frac{\partial^2 f}{\partial r^2}\right)_{j+\frac{1}{2}} \left(\frac{r_j}{2}\right)^2 + O(r_j^3) \quad , \tag{37}$$

where $\frac{1}{2}\, r_j$ is the distance from the cell center to the boundary and $O(r_j^3)$ indicates that the next term in the expansion is of order r_j^3. Similarly, we may write

$$f_{j+1} = f_{j+\frac{1}{2}} + \left(\frac{\partial f}{\partial r}\right)_{j+\frac{1}{2}} \frac{r_{j+1}}{2} + \frac{1}{2}\left(\frac{\partial^2 f}{\partial r^2}\right)_{j+\frac{1}{2}} \left(\frac{r_{j+1}}{2}\right)^2 + O(r_{j+1}^3) \quad . \tag{38}$$

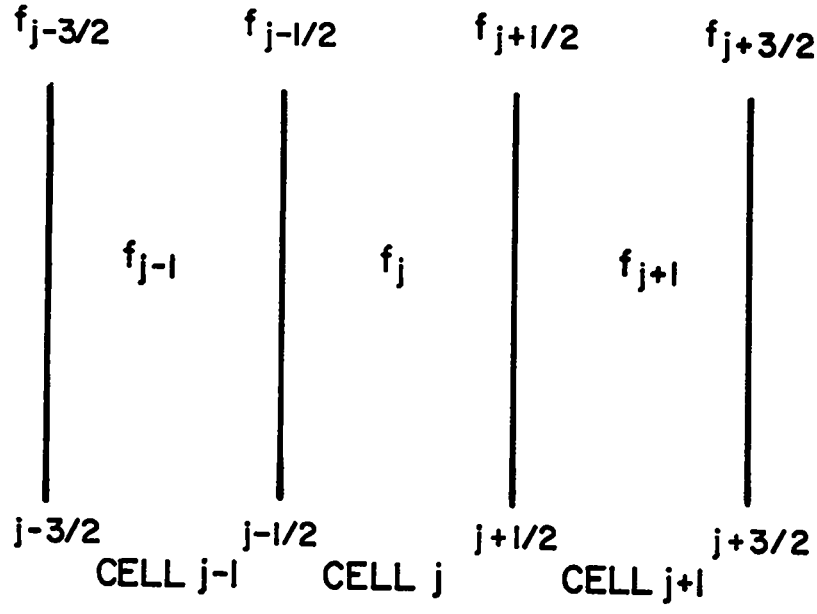


Fig. 7.
A function f evaluated on a Lagrangian coordinate system in one dimension. Integer values of the subscript denote cell centers and half-integer values denote cell boundaries.

Subtracting Eq. (37) from Eq. (38), we obtain the desired result:

$$f_{j+1} - f_j = \frac{1}{2}\left(\frac{\partial f}{\partial r}\right)_{j+\frac{1}{2}} (r_j + r_{j+1}) + O(r^2) \quad ,$$

$$\left(\frac{\partial f}{\partial r}\right)_{j+\frac{1}{2}} \cong \frac{(f_{j+1} - f_j)}{\frac{1}{2}(r_{j+1} + r_j)} + O(r) \quad . \tag{39}$$

If we multiply Eq. (37) by r_{j+1}, Eq. (38) by r_j, and add, we get

$$r_{j+1} f_j + r_j f_{j+1} = r_{j+1} f_{j+\frac{1}{2}} + r_j f_{j+\frac{1}{2}} + O(r^3) \quad ,$$

$$f_{j+\frac{1}{2}} \cong \frac{r_{j+1} f_j + r_j f_{j+1}}{r_j + r_{j+1}} + O(r^2) \quad . \tag{40}$$

This result gives us the value of a function at the boundary between two cells knowing only the values at the adjacent cell centers.

To obtain the derivative of a function at the cell center, we make a different expansion:

$$f_{j+\frac{1}{2}} = f_j + \left(\frac{\partial f}{\partial r}\right)_j \frac{r_j}{2} + \frac{1}{2}\left(\frac{\partial^2 f}{\partial r^2}\right)_j \left(\frac{r_j}{2}\right)^2 + O(r_j^3) \quad ,$$

$$f_{j-\frac{1}{2}} = f_j - \left(\frac{\partial f}{\partial r}\right)_j \frac{r_j}{2} + \frac{1}{2}\left(\frac{\partial^2 f}{\partial r^2}\right)_j \left(\frac{r_j}{2}\right)^2 + O(r_j^3) \quad .$$

Subtracting,

$$f_{j+\frac{1}{2}} - f_{j-\frac{1}{2}} = \left(\frac{\partial f}{\partial r}\right)_j r_j + O(r_j^3)$$

or

$$\left(\frac{\partial f}{\partial r}\right)_j = \frac{f_{j+\frac{1}{2}} - f_{j-\frac{1}{2}}}{r_j} + O(r_j^2) \quad . \tag{41}$$

The results of this section (Eqs. (39)-(41)) will be used to obtain the finite difference form of the equations of motion. As will be seen, we will have information about different quantities at different Lagrangian positions (cell centers or boundaries) and must use the results of this section to evaluate the function or its derivatives where they are needed.

2. Space and Time Grid

In writing down the finite difference solutions for the differential equations of motion, we must make some decisions about where in the space-time grid the various dynamic and thermodynamic quantities should be evaluated. Any choice we make will not be unique. Figure 8 illustrates the space-time grid we will be using. Cell j has boundaries at $j\pm\frac{1}{2}$ and we associate with the center of the cell the density (or volume), mass, stress, total energy, and internal energy.

V_j = volume of cell j $(V = \rho^{-1})$

M_j = mass of cell j (Lagrangian variable)*

ρ_j = density of cell j

σ_j = stress of cell j

E_j = total energy of cell j

I_j = internal energy of cell j

We locate the positions, R, of the cell boundaries at $j\pm\frac{1}{2}$ as measured in the laboratory coordinate frame. This also locates the velocities at the boundaries.

$R_{j+\frac{1}{2}}$ = position of one boundary of cell j

$u_{j+\frac{1}{2}} = \frac{\partial R_{j+\frac{1}{2}}}{\partial t}$ = velocity of one boundary of cell j

*M_j is equivalent to the differential mass element dm introduced in Sec. III.A; that is, $dm = M_j$.

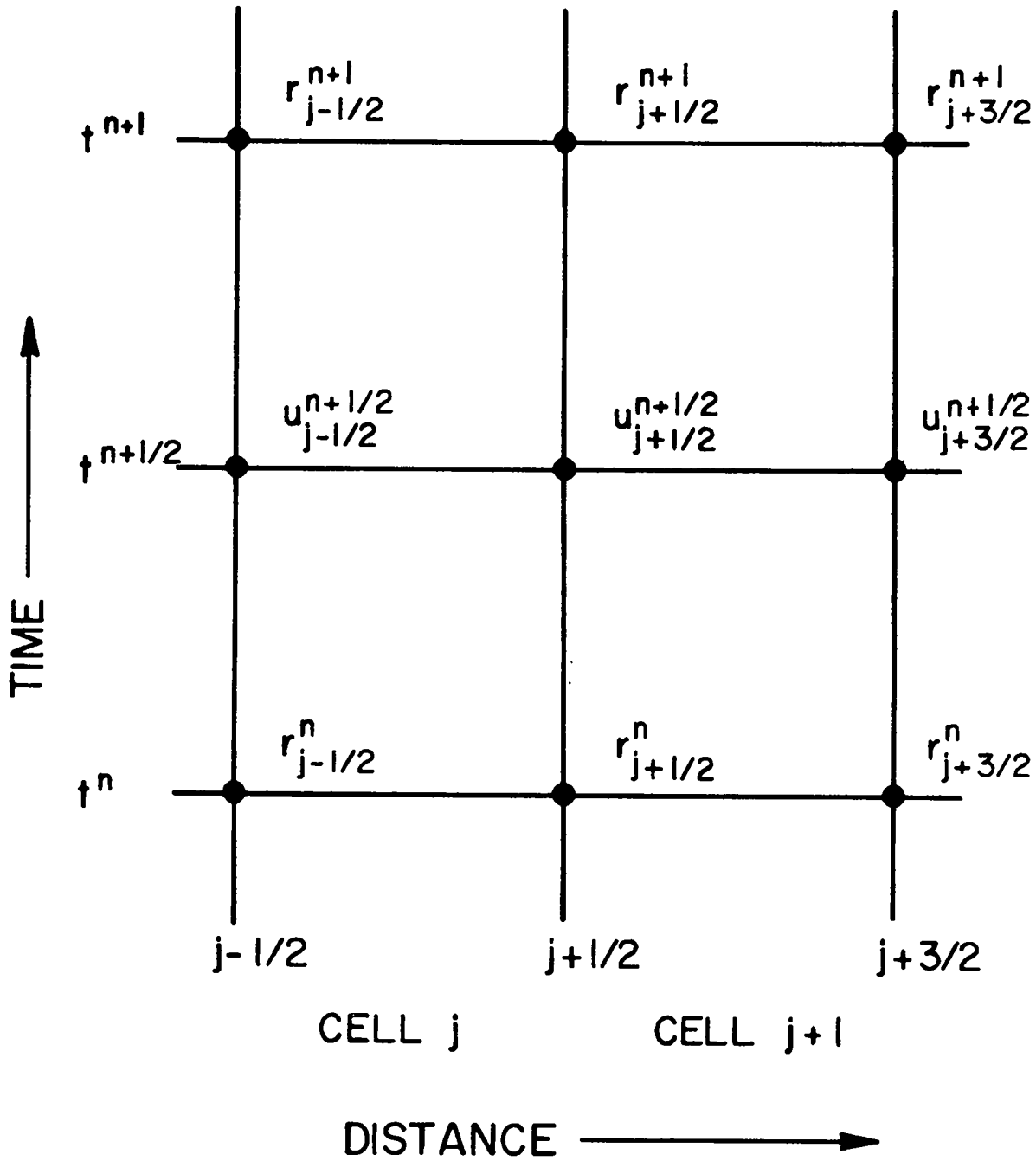


Fig. 8.
Space-time grid for the evaluation of cell quantities as used in HYDROX.

The choice of the time grid is slightly more difficult and we introduce the notion of a "half time step" to avoid confusion. By inspection of Eq. (39) of the previous section, assuming that we replace the spatial variable j by the time variable n, we see that knowing a quantity at time t = n and t = n+1 allows a straightforward determination of derivatives at t = n+½. The same argument applies for quantities known at t = n+½ and t = n+3/2 when we need to evaluate derivatives at t = n+1. Thus, we make the following choices at integer values of n (indicated by a superscript):

$$R_{j+\frac{1}{2}}^{n},\ V_{j}^{n},\ \rho_{j}^{n},\ \sigma_{j}^{n},\ E_{j}^{n},\ I_{j}^{n} \quad .$$

At half-integer values of n we choose

$$u_{j+\frac{1}{2}}^{n+\frac{1}{2}} \quad .$$

The mass of cell j, M_j, is a constant in time and does not need the time superscript.

The velocity is given by

$$u_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \left(\frac{\partial R}{\partial t}\right)_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{R_{j+\frac{1}{2}}^{n+1} - R_{j+\frac{1}{2}}^{n}}{\Delta t^{n}} + O(\Delta t^{2}) \quad ,$$

($O(\Delta t^2)$ means order of Δt squared; not to be confused with Δt^n meaning the value of the time step for the n^{th} cycle) which can be rewritten to give the position of the cell boundary at t = n+1, knowing the position at t = n and the velocity at t = n+½:

$$R_{j+\frac{1}{2}}^{n+1} = R_{j+\frac{1}{2}}^{n} + u_{j+\frac{1}{2}}^{n+1}\,\Delta t^{n} + O(\Delta t^{3}) \quad . \tag{42}$$

The volume of a cell can be calculated from a knowledge of the boundaries and the relation

$$dm = \rho\, r^{(d-1)}\, dr \quad ,$$

where d is the dimension (1, 2, or 3). Integrating both sides over a single cell of mass M_j, density ρ_j, from $R_{j-\frac{1}{2}}$ to $R_{j+\frac{1}{2}}$, we get

$$M_j = \rho_j \int_{R_{j-\frac{1}{2}}}^{R_{j+\frac{1}{2}}} r^{(d-1)}\, dr = \frac{\rho_j}{d}\left(R^d_{j+\frac{1}{2}} - R^d_{j-\frac{1}{2}}\right) \quad .$$

Using $V_j = \rho_j^{-1}$, we obtain for $t = n$

$$V_j^n = \frac{1}{M_j}\frac{1}{d}\left[\left(R^n_{j+\frac{1}{2}}\right)^d - \left(R^n_{j-\frac{1}{2}}\right)^d\right] \quad .$$

3. Momentum Equation

We want to write

$$\left(\frac{\partial u}{\partial t}\right)_r = -\left(\frac{\partial \sigma}{\partial m}\right)_t$$

in finite difference form, or more specifically, evaluate

$$\left(\frac{\partial u}{\partial t}\right)^n_{j+\frac{1}{2}} = -\left(\frac{\partial \sigma}{\partial m}\right)^n_{j+\frac{1}{2}} \quad .$$

For the left-hand side, we make Taylor series expansions of the velocity in time about $t = n$:

$$u^{n+\frac{1}{2}}_{j+\frac{1}{2}} = u^n_{j+\frac{1}{2}} + \left(\frac{\partial u}{\partial t}\right)^n_{j+\frac{1}{2}} \frac{\Delta t^n}{2} + \left(\frac{\partial^2 u}{\partial t^2}\right)^n_{j+\frac{1}{2}} \frac{(\Delta t^n)^2}{8} + O(\Delta t^3) \quad ,$$

$$u^{n-\frac{1}{2}}_{j+\frac{1}{2}} = u^n_{j+\frac{1}{2}} - \left(\frac{\partial u}{\partial t}\right)^n_{j+\frac{1}{2}} \frac{\Delta t^n}{2} + \left(\frac{\partial^2 u}{\partial t^2}\right)^n_{j+\frac{1}{2}} \frac{(\Delta t^n)^2}{8} - O(\Delta t^3) \quad .$$

Subtracting and solving for $(\partial u/\partial t)^n_{j+\frac{1}{2}}$, we get

$$\left(\frac{\partial u}{\partial t}\right)^n_{j+\frac{1}{2}} = \frac{u^{n+\frac{1}{2}}_{j+\frac{1}{2}} - u^{n-\frac{1}{2}}_{j+\frac{1}{2}}}{\Delta t^n} + O(\Delta t^2) \quad . \tag{43}$$

For the stress derivatives, expand σ^n_j and σ^n_{j+1} about the point $j+\frac{1}{2}$ and denote the Lagrangian incremental spatial variable dm by M_j:

$$\sigma^n_{j+1} = \sigma^n_{j+\frac{1}{2}} + \left(\frac{\partial \sigma}{\partial m}\right)^n_{j+\frac{1}{2}} \frac{M_{j+1}}{2} + O(M^2_{j+1}) \quad ,$$

$$\sigma^n_j = \sigma^n_{j+\frac{1}{2}} - \left(\frac{\partial \sigma}{\partial m}\right)^n_{j+\frac{1}{2}} \frac{M_j}{2} + O(M^2_j) \quad .$$

Subtracting and solving for $(\partial\sigma/\partial m)^n_{j+\frac{1}{2}}$, we get

$$-\left(\frac{\partial \sigma}{\partial m}\right)^n_{j+\frac{1}{2}} = -\frac{\sigma^n_{j+1} - \sigma^n_j}{\frac{1}{2}(M_{j+1} + M_j)} + O(\Delta M) \quad . \tag{44}$$

where $\Delta M = M_{j+1} - M_j$. Our final result obtained from Eqs. (43) and (44) is

$$\frac{u^{n+\frac{1}{2}}_{j+\frac{1}{2}} - u^{n-\frac{1}{2}}_{j+\frac{1}{2}}}{\Delta t^n} = \frac{\sigma^n_j - \sigma^n_{j+1}}{\frac{1}{2}(M_{j+1} + M_j)} + O(\Delta M) + O(\Delta t^2) \quad ,$$

which can be used to obtain the velocity at $t = n+\frac{1}{2}$ by knowing the stresses at $t = n$ to $O(\Delta M \Delta t)$ in the cell size and $O(\Delta t^3)$ in the time step.

$$u^{n+\frac{1}{2}}_{j+\frac{1}{2}} = u^{n-\frac{1}{2}}_{j+\frac{1}{2}} + \frac{\sigma^n_j - \sigma^n_{j+1}}{\frac{1}{2}(M_{j+1} + M_j)} \Delta t^n + O(\Delta M \Delta t) + O(\Delta t^3) \quad . \tag{45}$$

4. Energy Equation

The energy equation is

$$\left(\frac{\partial E}{\partial t}\right)_r = -\frac{\partial}{\partial m}(\sigma u) \quad .$$

In finite difference form, we will want to evaluate this equation at $t = n+\frac{1}{2}$ for mass element M_j:

$$\left(\frac{\partial E}{\partial t}\right)_j^{n+\frac{1}{2}} = -\left(\frac{\partial \sigma u}{\partial m}\right)_j^{n+\frac{1}{2}} \quad .$$

For the left-hand side, we make a Taylor series expansion about $t = n+\frac{1}{2}$:

$$E_j^{n+1} = E_j^{n+\frac{1}{2}} + \left(\frac{\partial E}{\partial t}\right)_j^{n+\frac{1}{2}} \frac{\Delta t^n}{2} + \left(\frac{\partial^2 E}{\partial t^2}\right)_j^{n+\frac{1}{2}} \frac{(\Delta t^n)^2}{8} + O(\Delta t^3) \quad ,$$

$$E_j^{n} = E_j^{n+\frac{1}{2}} - \left(\frac{\partial E}{\partial t}\right)_j^{n+\frac{1}{2}} \frac{\Delta t^n}{2} + \left(\frac{\partial^2 E}{\partial t^2}\right)_j^{n+\frac{1}{2}} \frac{(\Delta t^n)^2}{8} - O(\Delta t^3) \quad .$$

Subtracting and solving for $(\partial E/\partial t)_j^{n+\frac{1}{2}}$, we get

$$\left(\frac{\partial E}{\partial t}\right)_j^{n+\frac{1}{2}} = \frac{E_j^{n+1} - E_j^n}{\Delta t^n} + O(\Delta t^2) \quad . \tag{46}$$

For the right-hand side, we note that the mass element $dm = M_j$, the j^{th} Lagrangian coordinate. Expanding σu, we get

$$(\sigma u)_{j+\frac{1}{2}}^{n+\frac{1}{2}} = (\sigma u)_j^{n+\frac{1}{2}} + \left(\frac{\partial \sigma u}{\partial m}\right)_j^{n+\frac{1}{2}} \frac{M_j}{2} + \left(\frac{\partial^2 \sigma u}{\partial m^2}\right)_j^{n+\frac{1}{2}} \frac{M_j^2}{8} + O(M_j^3) \quad ,$$

$$(\sigma u)_{j-\frac{1}{2}}^{n+\frac{1}{2}} = (\sigma u)_j^{n+\frac{1}{2}} - \left(\frac{\partial \sigma u}{\partial m}\right)_j^{n+\frac{1}{2}} \frac{M_j}{2} + \left(\frac{\partial^2 \sigma u}{\partial m^2}\right)_j^{n+\frac{1}{2}} \frac{M_j^2}{8} + O(M_j^3) \quad .$$

Subtracting and solving for the quantity of interest, we get

$$\left(\frac{\partial \sigma u}{\partial m}\right)_j^{n+\frac{1}{2}} = \frac{(\sigma u)_{j+\frac{1}{2}}^{n+\frac{1}{2}} - (\sigma u)_{j-\frac{1}{2}}^{n+\frac{1}{2}}}{M_j} + O(M_j^2) \quad . \tag{47}$$

We still have the task of evaluating $(\sigma u)_{j+\frac{1}{2}}^{n+\frac{1}{2}}$. This can be written as

$$(\sigma u)_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \sigma_{j+\frac{1}{2}}^{n+\frac{1}{2}} u_{j+\frac{1}{2}}^{n+\frac{1}{2}} \quad ,$$

and $u_{j+\frac{1}{2}}^{n+\frac{1}{2}}$ is calculated from Eq. (45). For the stress, we shall approximate the time evaluation by

$$\sigma_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{\sigma_{j+\frac{1}{2}}^{n} + \sigma_{j+\frac{1}{2}}^{n+1}}{2} + O(\Delta t^2)$$

$$= \sigma_{j+\frac{1}{2}}^{n} + \frac{1}{2}\left(\sigma_{j+\frac{1}{2}}^{n+1} - \sigma_{j+\frac{1}{2}}^{n}\right) \cong \sigma_{j+\frac{1}{2}}^{n} + O(\Delta t) \quad .$$

$\sigma_{j+\frac{1}{2}}^{n+1}$ will be evaluated later from the equation of state using the results for V_j^{n+1} and I_j^{n+1}.

To evaluate the stress at the cell interface, we use Eq. (40):

$$\sigma_{j+\frac{1}{2}}^{n} = \frac{M_{j+1}\sigma_j^n + M_j\sigma_{j+1}^n}{M_j + M_{j+1}} + O(M_j^2) \quad . \tag{48}$$

We can now write the result using Eqs. (46)-(48):

$$\frac{E_j^{n+1} - E_j^n}{\Delta t^n} = -\frac{1}{M_j}\left\{\left[\frac{M_{j+1}\sigma_j^n + M_j\sigma_{j+1}^n}{M_j + M_{j+1}}\right]u_{j+\frac{1}{2}}^{n+\frac{1}{2}} - \left[\frac{M_j\sigma_{j-1}^n + M_{j-1}\sigma_j^n}{M_{j-1} + M_j}\right]u_{j-\frac{1}{2}}^{n+\frac{1}{2}}\right\}$$

$$+ O(M_j^2) + O(\Delta t) \quad . \tag{49}$$

This equation can then be used to solve for E_j^{n+1}.

5. Kinetic and Internal Energies

We shall define the internal energy I_j by the relations

$$E_j^{n+1} = I_j^{n+1} + \frac{1}{2}\left(u_j^{n+\frac{1}{2}}\right)^2 \quad , \tag{50}$$

$$E_j^{n} = I_j^{n} + \frac{1}{2}\left(u_j^{n-\frac{1}{2}}\right)^2 \quad . \tag{51}$$

To calculate $u_j^{n+\frac{1}{2}}$, we expand about j to get

$$u_{j+\frac{1}{2}}^{n+\frac{1}{2}} = u_j^{n+\frac{1}{2}} + \left(\frac{\partial u}{\partial m}\right)_j^{n+\frac{1}{2}} \frac{M_j}{2} + O(M_j^2) \quad ,$$

$$u_{j-\frac{1}{2}}^{n+\frac{1}{2}} = u_j^{n+\frac{1}{2}} - \left(\frac{\partial u}{\partial m}\right)_j^{n+\frac{1}{2}} \frac{M_j}{2} + O(M_j^2) \quad .$$

Adding gives

$$u_j^{n+\frac{1}{2}} = \frac{1}{2}\left(u_{j+\frac{1}{2}}^{n+\frac{1}{2}} + u_{j-\frac{1}{2}}^{n+\frac{1}{2}}\right) + O(M_j^2) \quad .$$

Substituting the result in Eqs. (50) and (51), combining with Eq. (49), and solving for I_j^{n+1}, we get

$$\begin{aligned} I_j^{n+1} = {} & I_j^n + \frac{1}{8}\left(u_{j+\frac{1}{2}}^{n+\frac{1}{2}} + u_{j-\frac{1}{2}}^{n+\frac{1}{2}}\right)^2 - \frac{1}{8}\left(u_{j+\frac{1}{2}}^{n-\frac{1}{2}} + u_{j-\frac{1}{2}}^{n-\frac{1}{2}}\right)^2 \\ & + \frac{\Delta t^n}{M_j}\left\{\left[\frac{M_j \sigma_{j-1}^n + M_{j-1}\sigma_j^n}{M_{j-1} + M_j}\right] u_{j-\frac{1}{2}}^{n+\frac{1}{2}} - \left[\frac{M_{j+1}\sigma_j^n + M_j \sigma_{j+1}^n}{M_j + M_{j+1}}\right] u_{j+\frac{1}{2}}^{n+\frac{1}{2}}\right\} \\ & + O(M_j^2 \Delta t) + O(\Delta t^2) \quad . \end{aligned} \tag{52}$$

This result is the expression used for the SIN difference equations.

For the HYDROX difference equation, the change in internal energy is calculated from the results of Sec. 4 above. In planar geometry, the time rate of change for the internal energy I is given by

$$\left(\frac{\partial I}{\partial t}\right)_r = -\sigma\left(\frac{\partial u}{\partial m}\right)_t \quad . \tag{53}$$

We can evaluate I_j^{n+1} by using a Taylor series expansion at t = n:

$$I_j^{n+1} = I_j^n + \Delta t^n\left(\frac{\partial I}{\partial t}\right)_j^n + O(\Delta t^2) \quad ,$$

which can be written, using Eq. (53), as

$$I_j^{n+1} = I_j^n - \Delta t^n \sigma_j^n\left(\frac{\partial u}{\partial m}\right)_j^n + O(\Delta t^2) \quad . \tag{54}$$

The derivative in Eq. (54) can be readily evaluated from Taylor series expansions about t = n and j:

$$u_{j+\frac{1}{2}}^{n+\frac{1}{2}} = u_{j+\frac{1}{2}}^n + \frac{\Delta t^n}{2}\left(\frac{\partial u}{\partial t}\right)_{j+\frac{1}{2}}^n + O(\Delta t^2) \quad , \tag{55}$$

$$u_{j+\frac{1}{2}}^{n-\frac{1}{2}} = u_{j+\frac{1}{2}}^n - \frac{\Delta t^n}{2}\left(\frac{\partial u}{\partial t}\right)_{j+\frac{1}{2}}^n + O(\Delta t^2) \quad , \tag{56}$$

$$u_{j+\frac{1}{2}}^n = u_j^n + \frac{M_j}{2}\left(\frac{\partial u}{\partial m}\right)_j^n + \frac{M_j^2}{8}\left(\frac{\partial^2 u}{\partial m^2}\right)_j^n + O(M_j^3) \quad , \tag{57}$$

$$u_{j-\frac{1}{2}}^n = u_j^n - \frac{M_j}{2}\left(\frac{\partial u}{\partial m}\right)_j^n + \frac{M_j^2}{8}\left(\frac{\partial^2 u}{\partial m^2}\right)_j^n + O(M_j^3) \quad . \tag{58}$$

Adding Eq. (55) and Eq. (56), we get

$$u_{j+\frac{1}{2}}^n = \frac{1}{2}\left(u_{j+\frac{1}{2}}^{n+\frac{1}{2}} + u_{j+\frac{1}{2}}^{n-\frac{1}{2}}\right) + O(\Delta t^2) \quad . \tag{59}$$

Subtracting Eq. (58) from Eq. (57) leads to

$$\left(\frac{\partial u}{\partial m}\right)_j^n = \frac{u_{j+\frac{1}{2}}^n - u_{j-\frac{1}{2}}^n}{M_j} + O(M_j^2) \quad . \tag{60}$$

Combining Eq. (59) and Eq. (60), we get

$$\left(\frac{\partial u}{\partial m}\right)_j^n = \frac{1}{2M_j}\left(u_{j+\frac{1}{2}}^{n+\frac{1}{2}} + u_{j+\frac{1}{2}}^{n-\frac{1}{2}} - u_{j-\frac{1}{2}}^{n+\frac{1}{2}} - u_{j-\frac{1}{2}}^{n-\frac{1}{2}}\right) + O(M_j^2) + O(\Delta t^2) \quad . \tag{61}$$

Inserting Eq. (61) in Eq. (54), we have the HYDROX difference equation for internal energy:

$$I_j^{n+1} = I_j^n - \frac{\Delta t^n \sigma_j^n}{2M_j}\left(u_{j+\frac{1}{2}}^{n+\frac{1}{2}} + u_{j+\frac{1}{2}}^{n-\frac{1}{2}} - u_{j-\frac{1}{2}}^{n+\frac{1}{2}} - u_{j-\frac{1}{2}}^{n-\frac{1}{2}}\right) + O(\Delta t^2) + O(M_j^2) \quad .$$

One can, at the expense of iterating on the equation of state, get a result for the internal energy with error $O(\Delta t^3)$ provided the velocities are calculated to $O(\Delta t^3)$. The error in Eq. (45) reduces to $O(\Delta t^3)$ for the special case of all M_j's equal. Future versions of HYDROX will include this iterative difference equation as an option.

6. Conservation Properties for the Difference Equations

In this section we shall investigate to what degree our difference equations conserve momentum and energy. To do this we sum the total momentum and energy of the system at two different times and compare the results. At $t = n+\frac{1}{2}$, the total momentum is

$$(Mu)^{n+\frac{1}{2}} = \sum_{j=0}^{N} \frac{1}{2}(M_j + M_{j+1})u_{j+\frac{1}{2}}^{n+\frac{1}{2}} \quad ,$$

where N is the number of cells. Using Eq. (45), we have

$$(Mu)^{n+\frac{1}{2}} = \sum_{j=0}^{N} \frac{1}{2}(M_j + M_{j+1})u_{j+\frac{1}{2}}^{n-\frac{1}{2}} + \sum_{j=0}^{N} \Delta t^n(\sigma_j^n - \sigma_{j+1}^n) + O(\Delta t^3) + O(\Delta M \Delta t)$$

$$= (Mu)^{n-\frac{1}{2}} + \Delta t^n \sum_{j=0}^{N} (\sigma_j^n - \sigma_{j+1}^n) + O(\Delta t^3) + O(\Delta M \Delta t)$$

$$= (Mu)^{n-\frac{1}{2}} + \Delta t^n\left[(\sigma_0^n - \sigma_1^n) + (\sigma_1^n - \sigma_2^n) + \cdots + (\sigma_{N-1}^n - \sigma_N^n) + (\sigma_N^n - \sigma_{N+1}^n)\right]$$
$$+ O(\Delta t^3) + O(\Delta M \Delta t)$$

$$= (Mu)^{n-\frac{1}{2}} + \Delta t^n(\sigma_0^n - \sigma_{N+1}^n) + O(\Delta t^3) + O(\Delta M \Delta t)$$

But the $j = 0$ and $j = N+1$ are effectively boundary cells that give free surface boundary conditions such that M_0 and $M_{n+1} = 0$ and $\sigma_0^n = \sigma_{N+1}^n = 0$ giving our conservation of momentum result,

$$(Mu)^{n+\frac{1}{2}} = (Mu)^{n-\frac{1}{2}} + O(\Delta t^3) + O(\Delta M \Delta t) \quad .$$

The total energy at $t = n+1$ is

$$(ME)^{n+1} = \sum_{j=1}^{N} M_j E_j^{n+1} \quad .$$

Using Eq. (49), we have for the SIN difference equations:

$$(ME)^{n+1} = \sum_{j=1}^{N} \left\{ M_j E_j^n + \Delta t^n \left(\left[\frac{M_j \sigma_{j-1}^n + M_{j-1}\sigma_j^n}{M_j + M_{j-1}} \right] u_{j-\frac{1}{2}}^{n+\frac{1}{2}} - \left[\frac{M_{j+1}\sigma_j^n + M_j \sigma_{j+1}^n}{M_j + M_{j+1}} \right] u_{j+\frac{1}{2}}^{n+\frac{1}{2}} \right) \right.$$
$$\left. + O(M_j \Delta t^2) \right\} \quad .$$

When the summation over j is performed, the first term is just the total energy at $t = n$. In the second term, let $k = j-1$ such that

$$\sum_{j=1}^{N} \rightarrow \sum_{k=0}^{N-1} \quad \text{and} \quad \begin{matrix} j \rightarrow k+1 \\ j-\tfrac{1}{2} \rightarrow k+\tfrac{1}{2} \end{matrix} \quad .$$

In a similar manner to the conservation of momentum calculation above, all terms cancel between the two summations except the k=0 term in the first summation and the j=N term in the second. Again, free surface boundary conditions give effective values of $M_0 = M_{N+1} = 0$ and $\sigma_0^n = \sigma_{N+1}^n = 0$ to obtain

$$(ME)^{n+1} = (ME)^n + O(M_j \Delta t^2) \quad .$$

Similarly, for the HYDROX difference equations, the conservation of total energy can be evaluated. The change in internal energy is given by

$$\Delta(MI) = \sum_{j=0}^{N} M_j (I_j^{n+1} - I_j^n)$$

$$= \sum_{j=0}^{N} M_j \sigma_j \frac{\left(u_{j-\frac{1}{2}}^{n+\frac{1}{2}} + u_{j-\frac{1}{2}}^{n-\frac{1}{2}} - u_{j+\frac{1}{2}}^{n+\frac{1}{2}} - u_{j+\frac{1}{2}}^{n-\frac{1}{2}}\right)\Delta t^n}{2M_j} + O(M_j \Delta t^2) + O(M_j^3) \quad ,$$

which can be rewritten as

$$\Delta(MI) = -\sum_{j=0}^{N} (\sigma_j^n - \sigma_{j+1}^n) \frac{1}{2}\left(u_{j+\frac{1}{2}}^{n+\frac{1}{2}} + u_{j+\frac{1}{2}}^{n-\frac{1}{2}}\right)\Delta t + O(M_j \Delta t^2) + O(M_j^3) \quad .$$

The change in kinetic energy can be written as

$$\Delta \frac{1}{2} Mu^2 = \frac{1}{2} \sum_{j=0}^{N} \frac{1}{2}(M_j + M_{j+1}) \left[\left(u_{j+\frac{1}{2}}^{n+\frac{1}{2}}\right)^2 - \left(u_{j+\frac{1}{2}}^{n-\frac{1}{2}}\right)^2\right] + O(M_j \Delta M \Delta t) \quad ,$$

which can be rewritten, using Eq. (45), to get

$$\Delta\left(\frac{1}{2} Mu^2\right) = \sum_{j=0}^{N} \left(\sigma_j^n - \sigma_{j+1}^n\right) \frac{1}{2}\left(u_{j+\frac{1}{2}}^{n+\frac{1}{2}} + u_{j+\frac{1}{2}}^{n-\frac{1}{2}}\right)\Delta t + O(M_j \Delta M \Delta t) \quad .$$

The total energy is then conserved to $O(M_j \Delta t^2) + O(M_j^3) + O(M_j \Delta M \Delta t)$.

III. INPUT AND OUTPUT

The input file for HYDROX is a namelist read file called DATA. HYDROX creates the following output files.

DOUT - a summary of all material and EOS constants for the entire problem

XOUT - the cycle print file

OUTPUT - a summary of material energies plus records of zoning, spalling, EOS errors, void closures, and restart dumps

GASSIN - random access graphics file ready to be processed by the LTSS utility GAS (LTSS-523)

DUMPO - a dump file for restarting a problem

Section A describes the variables for the input file DATA. Section B describes the output files. Section C tells how to process the GASSIN file for graphical output.

Defaults

The default value for all parameters listed in the namelist statements is 0 unless otherwise specified.

A. Namelist Input for the Input File DATA

Problem input to HYDROX is handled through the file DATA. The structure of the file is given by:

P$INP	Parameters for problem control	$	Required
P$SU	Parameters for Material 1	$	Required
P$ESC	EOS constants for Material 1	$	Required only if ME ≠ 0 in the SU namelist
P$BURN	Reactive EOS constants for Material 1	$	Required only if IBRN ≠ 0 in the ESC namelist or in data read from a library
P$SU	Parameters for Material 2	$	Required
P$ESC	EOS constants for Material 2	$	Required for ME ≠ 0
P$BURN	Reactive EOS constants for Material 2	$	Required for IBRN ≠ 0

Repeat SU, ESC, BURN for each material

1. Namelist INP

NM = number of material regions.

IALPH = 1,2,3, for plane, cylindrical, spherical geometry (default = 3).

LABEL = up to 80 characters of Hollerith data to be used as a label on the printout. Also, the first 30 characters will be used as a label on the GAS plots.

TEND = ending time (if NI is large enough). For TEND = 0, no check for TEND is made.

NI = maximum # of cycles the problem may run (default = 10000).

NDF = type of difference equations used. 1 = HYDROX, 2 = SIN (default = 1).

ND = approximate # of cells in the problem if the automatic zoner is used (default = 180).

MSFF = flag to use Multiple-Shock Forest Fire (MSFF = 1) instead of the usual Forest Fire (default).

PRINT and GASSIN Dump Controls

NP = print every NP cycles. For NP $\leq$ 0, no check for cycle print is made.

NG = GAS dump every NG cycles. For NG $\leq$ 0, no check for cycle GAS dump is made.

TP = $t_1,\Delta t_1,t_2,\Delta t_2,\cdots,\Delta t_{n-1},t_n$; print every Δt_1 μs from t_1 to t_2, every Δt_2 from t_2 to t_3, etc. (must end with t_n, not Δt_n). For $\Delta t \leq 0$, no check for time prints is made.

TG = same as TP except for GAS dump instead of print.

Automatic Time Step Parameters

NDELT = 0 for automatic time step control; 1 for Δt = DTO of the last active material region.

DTCF = automatic time step control parameter; Δt = DTCF* $\Delta X/C$ for all materials (see SU namelist).

Active Cell Control Parameters

NADD = add NADD new cells when the last cell becomes active.

NMAX = # of cells used initially (for NADD $\leq$ 0, all cells are used).

Piston Boundary Conditions

UI = initial piston velocity for HE initiation (no piston if UI = 0).

UF = final piston velocity for HE initiation.

RO = initial radius for piston.

UII = same as UI except for inside piston rather than outside piston.

UFI = same as UF except for inside piston rather than outside piston.

Restart Control Parameters

NM1 = minimum region # for which data will be read in (default = 1). Used primarily for a restart in which regions NM1 to NM are changed or added. If NM1 = 1 for a restart, no new data is read in except for that in the INP namelist.

IDMP = restart the problem at the IDMPth dump. If IDMP = 0, initialize problem from the data set.

IV = see SU namelist. Used in INP namelist only for restart with NM1 > 1 where IV(NM1-1) is set. (Default = -1.)

NDUMP = make a restart dump every NDUMP cycles. After MXDUMP (set in parameter statement, usually = 30) dumps, the code will stop. (Default = 10,000.)

TD = same as TP except for restart dumps.

SESAME Interpolation Option

IFN = 0 for rational function algorithm (default), 1 for bilinear algorithm.

2. Namelist SU

EOS Specifications

IEOS = type of EOS: 1 = HOM, 2 = buildup, 3 = 8-parameter fit, 4 = SESAME (default = 1).

MAT = EOS number in library for that type of EOS. A library is not searched if MAT = 0.

ME = 0 for no changes in library values, 1 for library values changed by the ESC (and sometimes BURN) namelist(s). ME must be 1 if MAT = 0.

Initial Positions and Velocity

R1 = outside radius for this material region (default = R0 for the first region; default = R2 of the previous region for other regions).

R2 = inside radius for this material region (required).

U0 = initial velocity for each cell in this region.

Zoning

NCI = number of cells in this region (must be at least 2 if used).

DR1, DR2 } for NCI = 0 (default) and DR1 > 0, NCI and DR (for each cell) are computed using DR1 and DR2. DR1 is the cell size for the outside cell of the region and DR2 is approximately the cell size for the inside cell of the region. The cell size varies linearly with cell number and DR2 is adjusted so that an integer number of cells is required. For NCI = 0 and DR1 $\leq$ 0, an automatic zoning scheme (described in SETUP) is used.

NOSPLT = 1 calculates and allows rezoning; $\leq$0 doesn't even check for rezoning.

Voids

IV = void index for the interface between this material and the next: -1 = no void (the two materials are "glued together" so that under tension they remain in contact), 0 = open void, +1 = closed void (which becomes an open void under tension)(default = -1).

Time-Step Controls

DTO = maximum allowed time step when this material region is the last active region. If DTO $\leq$ 0, it is replaced by DTO for the first region (which should not be 0). (Default = 1.)

DTCF = Automatic time-step control parameter for this material only; Δt = DTCF* $\Delta X/C$. (see DELT for details, default = 0.5).

Active Cell Control Parameters

UT = absolute value of the velocity that must be exceeded before the cell becomes active (default = 10^{-10}).

GAS Dump

IJK = GAS dumps. Include every IJK'th cell (default = 1).

3. Namelist ESC - Read Only if ME ≠ in the Immediately Preceding SU Namelist

ROW = initial density.

VO = initial volume.

PO = initial pressure.

XISP = pressure at which a closed void opens.

IE = initial region # (default, IE(I) = I).

QO = pressure at which viscosity is turned on (otherwise noise can make the problem unstable in regions where nothing should be happening) (default = 10^{-10}).

TO = initial temperature (for IEOS = 4 and TO ≠ 0, ZI (see below) is calculated using density and temperature as given quantities).

ZI = initial specific internal energy for all cells in a region.

HOM Parameters (IEOS = 1)
Library = HMLB

C1, S1 } C_0, S of $U_S = C_0 + SU_p$

C2, S2, SWV } second set of constants that are switched to when the volume is ≤SWV.

VMN = VMN < volume < SWV the volume is set to VMN in the EOS calculation.

GAMMA = Grüneisen γ (constant for HOM).

ALP = thermal expansion coefficient α used for HOM EOS in tension.

FS,GS,HS,SI,SJ = HOM parameters for the solid temperature fit (F,G,H,I,J).

CV = specific heat of the solid.

GC = array GC containing the HOM GAS constants (A,B,C,D,E,K,L,M,N,O,Q, R,S,T,U,C_V', and Z).

XL = thermal heat conductivity coefficient (not currently used).

XMU = μ = shear modulus.

YO = 2/3 Y_0.

PLAP = PLAP (see EPP).

TMLT = melt temperature at normal density.

TMC = melt constant for linear function of specific volume.

HOM Parameters for Reactive Materials

IBRN = type of burn: 0 = no burn, 1 = Arrhenius, 2 = CJ, 3 = sharp shock, 4 = Forest Fire. 5 = FF (temperature), 6 = FF (internal energy), 7 = gamma-law Taylor wave. If IBRN $\neq$ 0, the BURN namelist is read.

WO = initial burn fraction. Default = 1 - all solid, no products.

HE Buildup EOS (IEOS = 2)
Library = HMLB

BUA = A
BUB = B
BUMAX = γ_{max}
BUDV = D

where, for the detonation products, γ_g = A + B/X and X = distance from the detonation point, with the constraint $\gamma \leq \gamma_{max}$.

BUR = shift in effective distance of run.

BUD = region over which the "break" in γ is smoother (default = 0.2).

8-Parameter Polynomial Fits (IEOS = 3)

CF = 8-parameter EOS constants (see POLY).

SESAME EOS (IEOS = 4)
Library = SES2L

SR = density scale factor (default = 1).

ES = energy shift (Mbar - cm^3/g).

A1,A2,A3 = ramp parameters with a ramp pressure given by P = MIN{A1*(ρ/ρ_0 - 1), A2*(ρ/ρ_0 - A_3)}.

IRV = reversible (0)/irreversible flag (1).

EM = "melt" energy. For XI(J) > EM, a flag is set to turn off the ramp for that cell for the remainder of the problem.

Barnes EOS - Used with HOM

A,BR,BA,VBO,VBSW = constants used in Barnes EOS.

Spall Parameters - Used with HOM

SP = SPA in SIN (coefficient for the gradient spall pressure).

USP = ultimate spall pressure.

Viscosity Parameters

NV = viscosity type: 0 = "real," 1 = PIC (default), 2 = Landshoff.

XV = viscosity coefficient (default = 2.0).

4. Namelist BURN - Read Only if IBRN ≠ 0 in the Immediately Preceding ESC Namelist

Z = frequency for Arrhenius burn.

E = activation energy for Arrhenius burn.

VCJ = CJ volume for CJ burn.

PCJ = pressure at which W is set to 0 for Forest Fire burn.

DWDT = Forest Fire constants (up to 20).

PM = pressure below which dW/dt is assumed to be 0 for Forest Fire burn.

ND = # of Forest Fire constants.

SAMPLE DATA DECK

```
P$INP LABEL=50HSYMMETRIC PLATE IMPACT CU/CU
      NM=2,
      IALPH=1,
      TEND=4.,
      TP=0., 1., 4.0,
      TG=0., 0.5, 2., 0.1, 4.0,
      $
P$SU IEOS=1, MAT=4,
      R1=10., R2=9.,
      U0=-0.030,
      NCI=100
      $
P$SU IEOS=1, MAT=4,
      R2=8.,
      NCI=100,
      $
```

B. Output Files

In this section we present sample listings of the output files DOUT, XOUT, and OUTPUT. Two additional output files are also created during the execution of HYDROX: GASSIN for use by GAS, and DUMPO, a restart dump file.

1. DOUT. The file DOUT is written after the input namelists have been read and the problem has been set up. DOUT provides a means of checking and verifying the problem input. A sample DOUT listing is given in the following pages. The variables in the namelists INP, SU, and ESC are printed in the order they appear. See Section VI.A for a list of variables. Array variables are printed for all values of the array indices. Since many of the variables are dimensioned for the number of materials allowed, there can be many zeros. In the sample there were only 2 materials in the calculation, but HYDROX was compiled to allow 20.

SAMPLE DOUT LISTING

Begin Namelist INP

```
$INP    --

NM---------------------------------        2
UI---------------------------------   0.
UF---------------------------------   0.
RO---------------------------------   0.
IALPH------------------------------        1
NDF--------------------------------        1
NI---------------------------------    10000
NP---------------------------------        0
NG---------------------------------        0
NADD-------------------------------        0
NMAX-------------------------------      201
TEND-------------------------------   4.000000000000000E+00
TP(1)------------------------------   0.                    1.000000000000000E+00    4.000000000000000E+00
TP(4)------------------------------   0.                    0.                       0.
TP(7)------------------------------   0.                    0.                       0.
TP(10)-----------------------------   0.                    0.                       0.
TP(13)-----------------------------   0.                    0.                       0.
TP(16)-----------------------------   0.                    0.                       0.
TP(19)-----------------------------   0.                    0.                       0.
TG(1)------------------------------   0.                    5.000000000000000E-01    2.000000000000000E+00
TG(4)------------------------------   1.000000000000000E-01    4.000000000000000E+00    0.
TG(7)------------------------------   0.                    0.                       0.
TG(10)-----------------------------   0.                    0.                       0.
TG(13)-----------------------------   0.                    0.                       0.
TG(16)-----------------------------   0.                    0.                       0.
TG(19)-----------------------------   0.                    0.                       0.
NDELT------------------------------        0
UII--------------------------------   0.
UFI--------------------------------   0.
LABEL(1)---------------------------  **********  **********  **********          0          0          0          0
LABEL(8)---------------------------        0
NM1--------------------------------        1
IDMP-------------------------------        0
IV(1)------------------------------       -1         -1         -1         -1         -1         -1         -1
IV(8)------------------------------       -1         -1         -1         -1         -1         -1         -1
IV(15)-----------------------------       -1         -1         -1         -1         -1         -1         -1
IV(22)-----------------------------       -1         -1         -1         -1         -1         -1         -1
IV(29)-----------------------------       -1         -1         -1         -1         -1         -1         -1
IV(36)-----------------------------       -1         -1         -1         -1         -1         -1         -1
IV(43)-----------------------------       -1         -1         -1         -1         -1         -1         -1
IV(50)-----------------------------       -1         -1         -1         -1         -1         -1         -1
IV(57)-----------------------------       -1         -1         -1         -1         -1         -1         -1
IV(64)-----------------------------       -1         -1         -1         -1         -1         -1         -1
IV(71)-----------------------------       -1         -1         -1         -1         -1         -1         -1
IV(78)-----------------------------       -1         -1         -1         -1         -1         -1         -1
IV(85)-----------------------------       -1         -1         -1         -1         -1         -1         -1
IV(92)-----------------------------       -1         -1         -1         -1         -1         -1         -1
IV(99)-----------------------------       -1         -1
NDUMP------------------------------    10000
TD(1)------------------------------   0.                    0.                       0.
TD(4)------------------------------   0.                    0.                       0.
TD(7)------------------------------   0.                    0.                       0.
TD(10)-----------------------------   0.                    0.                       0.
TD(13)-----------------------------   0.                    0.                       0.
TD(16)-----------------------------   0.                    0.                       0.
TD(19)-----------------------------   0.                    0.                       0.
IFN--------------------------------        0
NO---------------------------------      180
DTCF(1)----------------------------   5.000000000000000E-01    5.000000000000000E-01    5.000000000000000E-01
DTCF(4)----------------------------   5.000000000000000E-01    5.000000000000000E-01    5.000000000000000E-01
DTCF(7)----------------------------   5.000000000000000E-01    5.000000000000000E-01    5.000000000000000E-01
```

```
DTCF(10)----------------------------  5.0000000000000E-01    5.0000000000000E-01    5.0000000000000E-01
DTCF(13)----------------------------  5.0000000000000E-01    5.0000000000000E-01    5.0000000000000E-01
DTCF(16)----------------------------  5.0000000000000E-01    5.0000000000000E-01    5.0000000000000E-01
DTCF(19)----------------------------  5.0000000000000E-01    5.0000000000000E-01    5.0000000000000E-01
$END
```

End Namelist INP

```
$SU     --
```

Begin Namelist SU

```
DTO(1)-------------------------------  1.0000000000000E+00    1.0000000000000E+00    1.0000000000000E+00
DTO(4)-------------------------------  1.0000000000000E+00    1.0000000000000E+00    1.0000000000000E+00
DTO(7)-------------------------------  1.0000000000000E+00    1.0000000000000E+00    1.0000000000000E+00
DTO(10)------------------------------  1.0000000000000E+00    1.0000000000000E+00    1.0000000000000E+00
DTO(13)------------------------------  1.0000000000000E+00    1.0000000000000E+00    1.0000000000000E+00
DTO(16)------------------------------  1.0000000000000E+00    1.0000000000000E+00    1.0000000000000E+00
DTO(19)------------------------------  1.0000000000000E+00    1.0000000000000E+00    1.0000000000000E+00
NOSPLT(1)----------------------------        0          0          0          0          0          0          0
NOSPLT(8)----------------------------        0          0          0          0          0          0          0
NOSPLT(15)---------------------------        0          0          0          0          0          0          0
NOSPLT(22)---------------------------        0          0          0          0          0          0          0
NOSPLT(29)---------------------------        0          0          0          0          0          0          0
NOSPLT(36)---------------------------        0          0          0          0          0          0          0
NOSPLT(43)---------------------------        0          0          0          0          0          0          0
NOSPLT(50)---------------------------        0          0          0          0          0          0          0
NOSPLT(57)---------------------------        0          0          0          0          0          0          0
NOSPLT(64)---------------------------        0          0          0          0          0          0          0
NOSPLT(71)---------------------------        0          0          0          0          0          0          0
NOSPLT(78)---------------------------        0          0          0          0          0          0          0
NOSPLT(85)---------------------------        0          0          0          0          0          0          0
NOSPLT(92)---------------------------        0          0          0          0          0          0          0
NOSPLT(99)---------------------------        0          0
IV(1)--------------------------------       -1         -1         -1         -1         -1         -1         -1
IV(8)--------------------------------       -1         -1         -1         -1         -1         -1         -1
IV(15)-------------------------------       -1         -1         -1         -1         -1         -1         -1
IV(22)-------------------------------       -1         -1         -1         -1         -1         -1         -1
IV(29)-------------------------------       -1         -1         -1         -1         -1         -1         -1
IV(36)-------------------------------       -1         -1         -1         -1         -1         -1         -1
IV(43)-------------------------------       -1         -1         -1         -1         -1         -1         -1
IV(50)-------------------------------       -1         -1         -1         -1         -1         -1         -1
IV(57)-------------------------------       -1         -1         -1         -1         -1         -1         -1
IV(64)-------------------------------       -1         -1         -1         -1         -1         -1         -1
IV(71)-------------------------------       -1         -1         -1         -1         -1         -1         -1
IV(78)-------------------------------       -1         -1         -1         -1         -1         -1         -1
IV(85)-------------------------------       -1         -1         -1         -1         -1         -1         -1
IV(92)-------------------------------       -1         -1         -1         -1         -1         -1         -1
IV(99)-------------------------------       -1         -1
IEOS(1)------------------------------        1          1          1          1          1          1          1
IEOS(8)------------------------------        1          1          1          1          1          1          1
IEOS(15)-----------------------------        1          1          1          1          1          1          1
MAT(1)-------------------------------        4          4          4          0          0          0          0
MAT(8)-------------------------------        0          0          0          0          0          0          0
MAT(15)------------------------------        0          0          0          0          0          0          0
ME(1)--------------------------------        1          1          1          0          0          0          0
ME(8)--------------------------------        0          0          0          0          0          0          0
ME(15)-------------------------------        0          0          0          0          0          0          0
R1-----------------------------------  8.0000000000018E+00
R2-----------------------------------  8.0000000000018E+00
UO(1)--------------------------------  -3.0000000000000E-02    0.                     0.
UO(4)--------------------------------  0.                     0.                     0.
UO(7)--------------------------------  0.                     0.                     0.
UO(10)-------------------------------  0.                     0.                     0.
UO(13)-------------------------------  0.                     0.                     0.
UO(16)-------------------------------  0.                     0.                     0.
UO(19)-------------------------------  0.                     0.                     0.
```

```
NCI----------------------------      100
DRI----------------------------  0.
DR2----------------------------  0.
UT(1)--------------------------  1.000000000000E-10   1.000000000000E-10   1.000000000000E-10
UT(4)--------------------------  1.000000000000E-10   1.000000000000E-10   1.000000000000E-10
UT(7)--------------------------  1.000000000000E-10   1.000000000000E-10   1.000000000000E-10
UT(10)-------------------------  1.000000000000E-10   1.000000000000E-10   1.000000000000E-10
UT(13)-------------------------  1.000000000000E-10   1.000000000000E-10   1.000000000000E-10
UT(16)-------------------------  1.000000000000E-10   1.000000000000E-10   1.000000000000E-10
UT(19)-------------------------  1.000000000000E-10   1.000000000000E-10   1.000000000000E-10
DTCF(1)------------------------  5.000000000000E-01   5.000000000000E-01   5.000000000000E-01
DTCF(4)------------------------  5.000000000000E-01   5.000000000000E-01   5.000000000000E-01
DTCF(7)------------------------  5.000000000000E-01   5.000000000000E-01   5.000000000000E-01
DTCF(10)-----------------------  5.000000000000E-01   5.000000000000E-01   5.000000000000E-01
DTCF(13)-----------------------  5.000000000000E-01   5.000000000000E-01   5.000000000000E-01
DTCF(16)-----------------------  5.000000000000E-01   5.000000000000E-01   5.000000000000E-01
DTCF(19)-----------------------  5.000000000000E-01   5.000000000000E-01   5.000000000000E-01
$END
```

End Namelist SU

```
$ESC    --
```

Begin Namelist ESC*

```
C1(1)--------------------------  3.958000000000E-01   3.958000000000E-01   3.958000000000E-01
C1(4)--------------------------  0.                   0.                   0.
C1(7)--------------------------  0.                   0.                   0.
C1(10)-------------------------  0.                   0.                   0.
C1(13)-------------------------  0.                   0.                   0.
C1(16)-------------------------  0.                   0.                   0.
C1(19)-------------------------  0.                   0.                   0.
S1(1)--------------------------  1.497000000000E+00   1.497000000000E+00   1.497000000000E+00
S1(4)--------------------------  0.                   0.                   0.
S1(7)--------------------------  0.                   0.                   0.
S1(10)-------------------------  0.                   0.                   0.
S1(13)-------------------------  0.                   0.                   0.
S1(16)-------------------------  0.                   0.                   0.
S1(19)-------------------------  0.                   0.                   0.
C2(1)--------------------------  0.                   0.                   0.
C2(4)--------------------------  0.                   0.                   0.
C2(7)--------------------------  0.                   0.                   0.
C2(10)-------------------------  0.                   0.                   0.
C2(13)-------------------------  0.                   0.                   0.
C2(16)-------------------------  0.                   0.                   0.
C2(19)-------------------------  0.                   0.                   0.
S2(1)--------------------------  0.                   0.                   0.
S2(4)--------------------------  0.                   0.                   0.
S2(7)--------------------------  0.                   0.                   0.
S2(10)-------------------------  0.                   0.                   0.
S2(13)-------------------------  0.                   0.                   0.
S2(16)-------------------------  0.                   0.                   0.
S2(19)-------------------------  0.                   0.                   0.
SWV(1)-------------------------  1.000000000000E-03   1.000000000000E-03   1.000000000000E-03
SWV(4)-------------------------  0.                   0.                   0.
SWV(7)-------------------------  0.                   0.                   0.
SWV(10)------------------------  0.                   0.                   0.
SWV(13)------------------------  0.                   0.                   0.
SWV(16)------------------------  0.                   0.                   0.
SWV(19)------------------------  0.                   0.                   0.
VMN(1)-------------------------  0.                   0.                   0.
VMN(4)-------------------------  0.                   0.                   0.
VMN(7)-------------------------  0.                   0.                   0.
VMN(10)------------------------  0.                   0.                   0.
VMN(13)------------------------  0.                   0.                   0.
VMN(16)------------------------  0.                   0.                   0.
VMN(19)------------------------  0.                   0.                   0.
```

*Not all variables in the ESC namelist are printed here since each variable is printed for all materials (20 allowed in this case) before going to the next variable.

2. XOUT. XOUT is the print file containing the cell dumps as controlled by either the NP or TP parameters in the INP namelist. Besides giving the cell quantities, the kinetic and internal energies by material and the problem totals are given at the beginning of each dump. This is the same information on material energies and problem totals that is contained on the OUTPUT file. A partial listing from a sample problem is given on the following page.

SAMPLE XOUT LISTING

SYMMETRIC PLATE IMPACT CU/CU

TIME= 4.00455E+00 DT= 1.26326E-02 CYCLE= 317

MATERIAL 1 ENERGY= 6.45511E-04 INTERNAL ENERGY= 4.10028E-04 KINETIC ENERGY= 2.35482E-04
MATERIAL 2 ENERGY= 3.34059E-03 INTERNAL ENERGY= 4.13702E-04 KINETIC ENERGY= 2.92689E-03
TOTAL ENERGY= 3.98610E-03 TOTAL INTERNAL ENERGY= 8.23730E-04 TOTAL KINETIC ENERGY= 3.16237E-03

J	IEOS	MAT	M	R	V	U	I	T	P	Q	SX	SZ	W
2	1	4	8.903E-02	9.928E+00	1.123E-01	-4.943E-04	6.664E-07	3.079E+02	-1.063E-07	1.887E-07	-5.470E-04	2.735E-04	1.000E+00
3	1	4	8.903E-02	9.918E+00	1.121E-01	-4.942E-04	9.704E-06	3.107E+02	-6.085E-07	2.860E-07	-2.998E-03	1.499E-03	1.000E+00
4	1	4	8.903E-02	9.908E+00	1.121E-01	-4.940E-04	1.487E-05	3.121E+02	-1.342E-06	1.243E-07	-2.995E-03	1.498E-03	1.000E+00
5	1	4	8.903E-02	9.898E+00	1.121E-01	-4.939E-04	1.762E-05	3.128E+02	-1.777E-06	5.713E-08	-2.999E-03	1.499E-03	1.000E+00
6	1	4	8.903E-02	9.888E+00	1.121E-01	-4.938E-04	1.872E-05	3.130E+02	-1.936E-06	0.	-2.999E-03	1.500E-03	1.000E+00
7	1	4	8.903E-02	9.878E+00	1.121E-01	-4.940E-04	1.871E-05	3.130E+02	-1.574E-06	0.	-2.999E-03	1.500E-03	1.000E+00
8	1	4	8.903E-02	9.868E+00	1.121E-01	-4.942E-04	1.788E-05	3.128E+02	-7.946E-07	0.	-2.999E-03	1.500E-03	1.000E+00
9	1	4	8.903E-02	9.858E+00	1.121E-01	-4.944E-04	1.830E-05	3.129E+02	7.702E-07	0.	-2.997E-03	1.499E-03	1.000E+00
10	1	4	8.903E-02	9.848E+00	1.121E-01	-4.945E-04	2.011E-05	3.134E+02	2.127E-06	1.536E-07	-2.997E-03	1.499E-03	1.000E+00
11	1	4	8.903E-02	9.838E+00	1.121E-01	-4.943E-04	2.124E-05	3.137E+02	3.157E-06	2.849E-07	-2.997E-03	1.499E-03	1.000E+00
12	1	4	8.903E-02	9.828E+00	1.121E-01	-4.941E-04	2.177E-05	3.138E+02	3.832E-06	2.972E-07	-2.997E-03	1.498E-03	1.000E+00
13	1	4	8.903E-02	9.818E+00	1.121E-01	-4.939E-04	2.199E-05	3.139E+02	4.130E-06	2.350E-07	-2.997E-03	1.498E-03	1.000E+00
14	1	4	8.903E-02	9.808E+00	1.121E-01	-4.937E-04	2.206E-05	3.139E+02	4.227E-06	1.727E-07	-2.997E-03	1.499E-03	1.000E+00
15	1	4	8.903E-02	9.798E+00	1.121E-01	-4.936E-04	2.211E-05	3.139E+02	4.415E-06	1.623E-07	-2.997E-03	1.498E-03	1.000E+00
16	1	4	8.903E-02	9.788E+00	1.121E-01	-4.935E-04	2.213E-05	3.139E+02	4.771E-06	1.621E-07	-2.998E-03	1.499E-03	1.000E+00
17	1	4	8.903E-02	9.778E+00	1.121E-01	-4.933E-04	2.214E-05	3.139E+02	5.085E-06	1.211E-07	-2.996E-03	1.498E-03	1.000E+00
18	1	4	8.903E-02	9.768E+00	1.121E-01	-4.933E-04	2.216E-05	3.139E+02	5.154E-06	4.327E-08	-2.997E-03	1.499E-03	1.000E+00
19	1	4	8.903E-02	9.758E+00	1.121E-01	-4.932E-04	2.217E-05	3.139E+02	4.885E-06	0.	-2.998E-03	1.499E-03	1.000E+00
20	1	4	8.903E-02	9.748E+00	1.121E-01	-4.933E-04	2.218E-05	3.139E+02	4.362E-06	0.	-2.998E-03	1.499E-03	1.000E+00
21	1	4	8.903E-02	9.738E+00	1.121E-01	-4.934E-04	2.219E-05	3.139E+02	4.011E-06	0.	-2.998E-03	1.499E-03	1.000E+00
22	1	4	8.903E-02	9.728E+00	1.121E-01	-4.935E-04	2.220E-05	3.139E+02	2.969E-06	0.	-2.998E-03	1.499E-03	1.000E+00
23	1	4	8.903E-02	9.718E+00	1.121E-01	-4.938E-04	2.220E-05	3.139E+02	2.029E-06	0.	-2.999E-03	1.500E-03	1.000E+00
24	1	4	8.903E-02	9.708E+00	1.121E-01	-4.942E-04	2.221E-05	3.139E+02	1.882E-06	0.	-2.999E-03	1.500E-03	1.000E+00
25	1	4	8.903E-02	9.698E+00	1.121E-01	-4.945E-04	2.222E-05	3.139E+02	1.748E-06	0.	-2.999E-03	1.499E-03	1.000E+00
26	1	4	8.903E-02	9.688E+00	1.121E-01	-4.948E-04	2.223E-05	3.139E+02	1.799E-06	0.	-3.000E-03	1.500E-03	1.000E+00
27	1	4	8.903E-02	9.678E+00	1.121E-01	-4.948E-04	2.224E-05	3.139E+02	1.844E-06	6.353E-08	-3.000E-03	1.500E-03	1.000E+00
28	1	4	8.903E-02	9.668E+00	1.121E-01	-4.948E-04	2.224E-05	3.139E+02	1.451E-06	2.645E-07	-2.999E-03	1.500E-03	1.000E+00
29	1	4	8.903E-02	9.658E+00	1.121E-01	-4.946E-04	2.225E-05	3.139E+02	3.039E-07	0.	-2.999E-03	1.500E-03	1.000E+00
30	1	4	8.903E-02	9.648E+00	1.121E-01	-4.946E-04	2.226E-05	3.139E+02	-1.715E-06	0.	-3.000E-03	1.500E-03	1.000E+00
31	1	4	8.903E-02	9.638E+00	1.121E-01	-4.947E-04	2.227E-05	3.139E+02	-2.055E-06	4.162E-07	-3.000E-03	1.500E-03	1.000E+00
32	1	4	8.903E-02	9.628E+00	1.121E-01	-4.944E-04	2.227E-05	3.139E+02	-4.445E-07	5.810E-07	-2.999E-03	1.500E-03	1.000E+00
33	1	4	8.903E-02	9.618E+00	1.121E-01	-4.940E-04	2.228E-05	3.139E+02	4.906E-07	0.	-2.999E-03	1.500E-03	1.000E+00
34	1	4	8.903E-02	9.608E+00	1.121E-01	-4.941E-04	2.229E-05	3.139E+02	2.597E-06	3.884E-07	-2.998E-03	1.499E-03	1.000E+00
35	1	4	8.903E-02	9.598E+00	1.121E-01	-4.938E-04	2.229E-05	3.139E+02	2.452E-06	0.	-3.000E-03	1.500E-03	1.000E+00
36	1	4	8.903E-02	9.588E+00	1.121E-01	-4.944E-04	2.230E-05	3.139E+02	3.972E-06	2.711E-07	-3.000E-03	1.500E-03	1.000E+00
37	1	4	8.903E-02	9.578E+00	1.121E-01	-4.942E-04	2.231E-05	3.139E+02	1.547E-06	0.	-3.000E-03	1.501E-03	1.000E+00
38	1	4	8.903E-02	9.568E+00	1.121E-01	-4.960E-04	2.232E-05	3.139E+02	9.448E-06	0.	-3.000E-03	1.500E-03	1.000E+00
39	1	4	8.903E-02	9.558E+00	1.121E-01	-4.964E-04	2.232E-05	3.139E+02	1.359E-05	0.	-2.999E-03	1.500E-03	1.000E+00
			Mass	Radius	Volume	Velocity	Internal Energy	Temperature	Pressure	Viscosity	Stress Deviators		Mass Fraction

3. OUTPUT. The file OUTPUT contains a summary of the problem energies plus various other information about what happened during the problem execution. The following list contains the information that may be written to OUTPUT.

Number of zones in each material, EOS type and number, $\sqrt{\rho_0}\Delta r$ for the and outside cell.

Error messages for materials not in an EOS library.

Time, Δt, cycle, and energy sums by material and problem total (same as in XOUT).

Record of any dump written or read for a restart.

Record of any spalling.

Record of any HOM iteration errors for a mixture of solid and gas product.

Record of void collapses or openings.

Record of any iteration failures for high-velocity void collapses.

A sample OUTPUT file is listed on the following page. Information about EOS errors, spalling, etc. is listed only if they occur.

Material	# Zones	Type	EOS #	$\sqrt{\rho_0}\Delta r$ Outside Cell	$\sqrt{\rho_0}\Delta r$ Inside Cell
1	100	1	4	2.984E-02	2.984E-02
2	100	1	4	2.984E-02	2.984E-02

```
TIME=      0.          DT=  1.00000E+00 CYCLE=          0

 MATERIAL  1 ENERGY= 3.97630E-03 INTERNAL ENERGY= 0.          KINETIC ENERGY= 3.97630E-03
 MATERIAL  2 ENERGY= 0.          INTERNAL ENERGY= 0.          KINETIC ENERGY= 0.
 TOTAL ENERGY= 3.97630E-03 TOTAL INTERNAL ENERGY= 0.          TOTAL KINETIC ENERGY= 3.97630E-03

TIME=      1.26326E-02 DT=  1.26326E-02 CYCLE=          1

 MATERIAL  1 ENERGY= 3.97630E-03 INTERNAL ENERGY= 0.          KINETIC ENERGY= 3.97630E-03
 MATERIAL  2 ENERGY= 0.          INTERNAL ENERGY= 0.          KINETIC ENERGY= 0.
 TOTAL ENERGY= 3.97630E-03 TOTAL INTERNAL ENERGY= 0.          TOTAL KINETIC ENERGY= 3.97630E-03

TIME=      2.52653E-02 DT=  1.26326E-02 CYCLE=          2

 MATERIAL  1 ENERGY= 3.98155E-03 INTERNAL ENERGY= 1.86438E-05 KINETIC ENERGY= 3.96290E-03
 MATERIAL  2 ENERGY= 1.35924E-06 INTERNAL ENERGY= 1.77453E-16 KINETIC ENERGY= 1.35924E-06
 TOTAL ENERGY= 3.98291E-03 TOTAL INTERNAL ENERGY= 1.86438E-05 TOTAL KINETIC ENERGY= 3.96426E-03

TIME=      1.01061E+00 DT=  1.26326E-02 CYCLE=         80

 MATERIAL  1 ENERGY= 3.15778E-03 INTERNAL ENERGY= 4.42471E-04 KINETIC ENERGY= 2.71531E-03
 MATERIAL  2 ENERGY= 8.27660E-04 INTERNAL ENERGY= 4.26922E-04 KINETIC ENERGY= 4.00738E-04
 TOTAL ENERGY= 3.98544E-03 TOTAL INTERNAL ENERGY= 8.69393E-04 TOTAL KINETIC ENERGY= 3.11604E-03

TIME=      2.00859E+00 DT=  1.26326E-02 CYCLE=        159

 MATERIAL  1 ENERGY= 2.32025E-03 INTERNAL ENERGY= 8.69209E-04 KINETIC ENERGY= 1.45104E-03
 MATERIAL  2 ENERGY= 1.66530E-03 INTERNAL ENERGY= 8.53659E-04 KINETIC ENERGY= 8.11641E-04
 TOTAL ENERGY= 3.98555E-03 TOTAL INTERNAL ENERGY= 1.72287E-03 TOTAL KINETIC ENERGY= 2.26268E-03

TIME=      3.00657E+00 DT=  1.26326E-02 CYCLE=        238

 MATERIAL  1 ENERGY= 1.48288E-03 INTERNAL ENERGY= 7.91417E-04 KINETIC ENERGY= 6.91463E-04
 MATERIAL  2 ENERGY= 2.50313E-03 INTERNAL ENERGY= 7.95195E-04 KINETIC ENERGY= 1.70793E-03
 TOTAL ENERGY= 3.98601E-03 TOTAL INTERNAL ENERGY= 1.58661E-03 TOTAL KINETIC ENERGY= 2.39940E-03
DUMP   1 AT CYCLE       317,TIME=  .40045E+01

TIME=      4.00455E+00 DT=  1.26326E-02 CYCLE=        317

 MATERIAL  1 ENERGY= 6.45511E-04 INTERNAL ENERGY= 4.10028E-04 KINETIC ENERGY= 2.35482E-04
 MATERIAL  2 ENERGY= 3.34059E-03 INTERNAL ENERGY= 4.13702E-04 KINETIC ENERGY= 2.92689E-03
 TOTAL ENERGY= 3.98610E-03 TOTAL INTERNAL ENERGY= 8.23730E-04 TOTAL KINETIC ENERGY= 3.16237E-03
```

4. GASSIN. GASSIN is a random access file written in the MAGEE Movie format for direct processing by the graphics utility GAS (LTSS-523). The structure of GASSIN consists of a file index that is 1003_{10} words long and dumps for each specified problem time.

File Index

Disk Address	Word	Contents	
0	1	Integer giving the number of words in the index	
1	2	Integer giving the number of dumps in this file	
2	3	Disk address of the last word in this file	
3	4	Problem dump time for the first dump	1
4	5	Disk address for the first dump in this file	1
5	6	Problem dump time for the second dump	2
6	7	Disk address for the second dump in this file	2
		.	
		.	
		.	
		Repeat dump time, disk address for each dump	

Data Dumps

Each data dump consists of two parts. The first 100 words contain information about the data in the dump. The data begins at word 101 after the beginning of the data dump and is packed three HYDROX cell variables per word (see GAS writeup). The contents of the first 100 words are as follows.
(I = integer, F = floating point, H = Hollerith. Omitted numbers are not used.)

Word	Contents
1	Dump Time (F)
2	The number of zones for the problem (I)
3	1 (I)
4	Not used
5	Number of packed words per cell = 4 (I)
6	Number of cell variables per word = 3 (I)
⋮	
10	Number of fraction bits in the packing format = 14 (I)
11	Number of exponent bits in the packing format = 5 (I)
⋮	
81	Date (H)
⋮	
90	Problem label, first 10 characters (H)
91	Problem label, second 10 characters (H)
92	Problem label, third 10 characters (H)
93	First value of the cell number = 1 (I)
94	1 (I)

5. DUMPO. A restart capability is provided by the writing and reading of the dump file DUMPO. The frequency of dumps may be selected by either specifying the problem time or cycle number. The problem geometry may also be changed, adding or deleting zones, materials, equation-of-state parameters, or anything capable of being specified in the original problem setup. A description of the control variables is given in the "Restart Control Parameters" of Sec. III.A.1, Namelist INP. Further details are provided in the descriptions of subroutines WDUMP and RDUMP of Sec. IV, HYDROX Description by Subroutines.

C. Graphics

The graphical output file GASSIN is written in a random access MAGEE movie format for processing by the LTSS utility GAS (LTSS-523). GAS allows the users to make plots of all cell quantities as a function of distance or any other cell variable. In addition, time plots of cell quantities and contour plots in position-time (X-t) space can be made. GAS can be run as an interactive utility or through a controller.

The variable numbers used by GAS and their corresponding HYDROX quantities are given by:

Gas Variable Number	1	2	3	4	5	6	7	8	9	10	11	12
Cell Quantity	region index	t	r	u	V	I	P	S_X	S_Z (or W if $\mu = 0$)	EE*	T	q

*The variable EE contains energy sums in cell quantities in the following order:

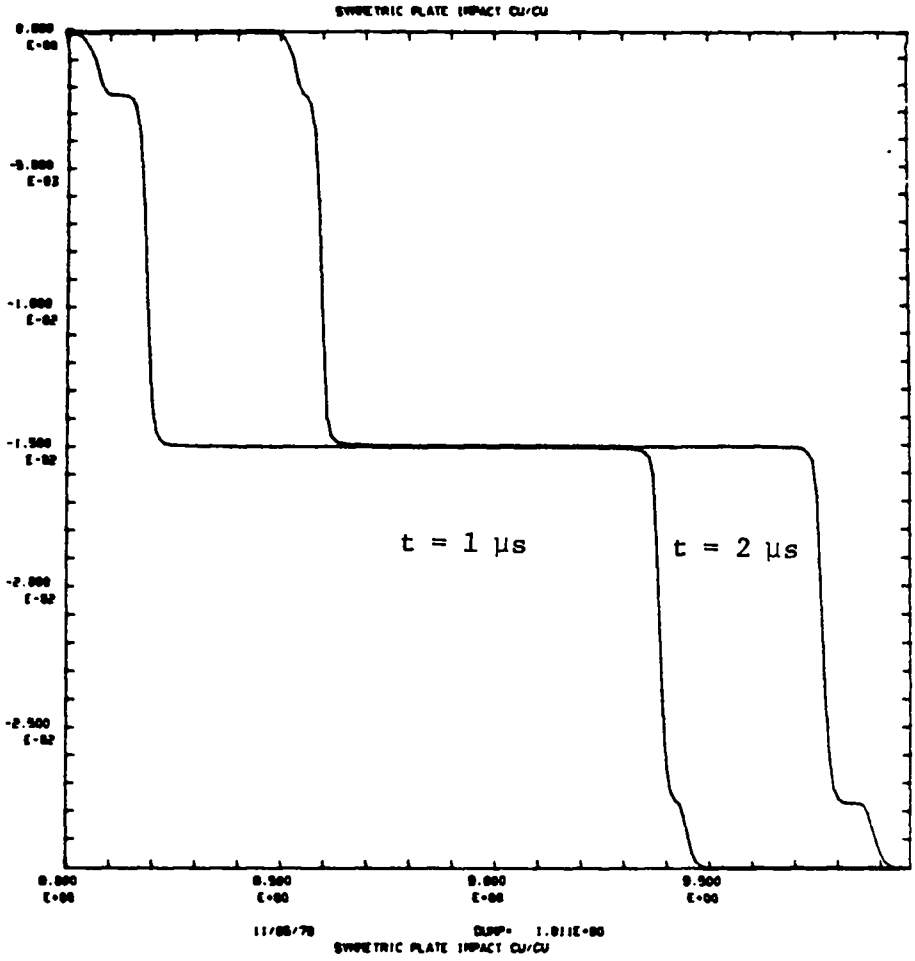
1 to ML-1	total energy for region 1 to ML-1
ML	total energy for the problem plus work done on pistons
ML+1 to 2*ML-1	internal energy for region 1 to ML-1
2*ML	total internal energy for the problem
2*ML+1 to 3*ML-1	kinetic energy for region 1 to ML-1
3*ML	total kinetic energy for the problem
4*ML+1	work done on the outside piston
4*ML+2	work done on the inside piston

ML is set in a parameter statement and is usually 21, the number of allowed materials plus one.

The sample GAS plots on the following page were generated by the commands listed below.

GAS!GASSIN!YES!ME	Initialize GAS and enter the MESH plot mode
DC,3,4!SR!DU,1!	Plot the particle velocity vs radius and allow GAS to select a rectangle to plot the data; the dump at time = 1 μs was specified
DU,2!MP!	Plot the particle velocity vs radius at time = 2 μs and overlay it on the previous graph
CV,3,7!SR!DU,1!	Plot the pressure vs radius for time = 1 μs
DU,2!MP!	Plot the pressure vs radius at time = 2 μs and overlay it on the previous graph
END	Terminate the execution of GAS

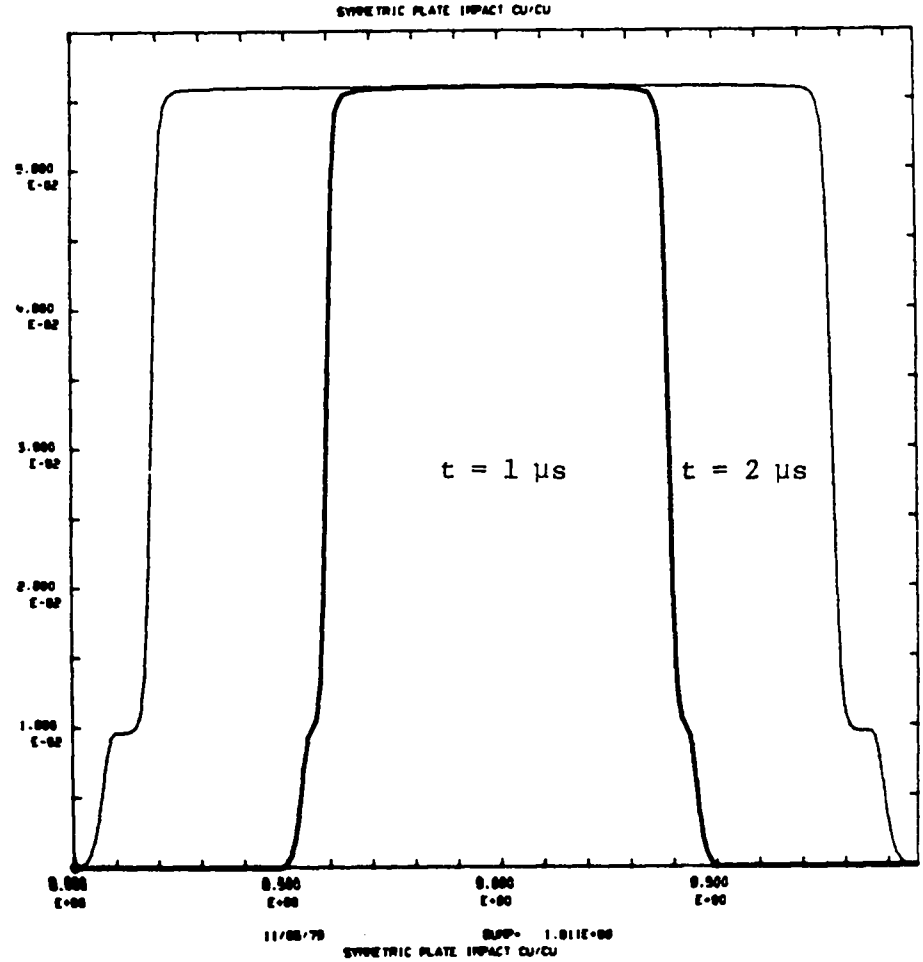
Velocity
vs
Radius
(CV,3,4)



Sample

Gas Plots

Pressure
vs
Radius
(DV,3,7)



IV. HYDROX DESCRIPTION BY SUBROUTINES

This section contains the most detailed information about the inner workings of HYDROX. Part A contains a summary description of each subroutine and Part B contains a logical flow diagram. Part C contains further information about each subroutine by first giving an annotated FORTRAN listing and then giving detailed notes on local variables, relevant physical models, and numerical algorithms.

A. Summary Description of the Subroutines

MAIN

Calls routines to set up the problem.

Contains the main cycle loop of the code which checks whether to add cells, print, make a GAS dump, make a restart dump, or end the problem; calls subroutines to rezone if necessary, determine the time step, and run one hydro cycle.

SETUP

Controls the setup of the problem, reads INP namelist, checks for a restart dump, calls other routines to read the rest of the namelists data from EOS files, initializes all of the cell quantities except pressure, writes out all variables in all namelists to the file DOUT.

SSU

Reads the SU namelist and copies material data to region I+1. In order to keep the namelist variable names the same as those used in the code and at the same time avoid requiring region number subscripts in the input, region number one (i.e., no subscript) is used in the namelist. The data is then copied to region number I+1 where I is the actual region number. After all data is read in, every variable associated with regions has all of its data shifted down by one to the proper region. See subroutine RSTORE.

ESSU

Reads the ESC namelist (equation-of-state constants) and copies material data to region I+1.

BRSU

Reads the BURN namelist (various burn constants) and copies material data to region I+1.

CLR

Resets region 1 data to the default values.

RSTORE

Shifts region I+1 data back to I (where it should be) for each region I.

EOSDSK

Switching routine that assigns units for EOS files and calls routines to read them. Data from EOS files can then be overridden by namelist reads.

RHOM

Reads EOS file HMLB to get HOM EOS data.

RBLDUP

Reads EOS file HMLB to get data for the buildup EOS and burn model.

RPOLY

Dummy routine because a library is not provided for the eight-parameter fit constants.

RSESAME

Reads data from disk for SESAME materials.

JMNMX

Sets indices to determine the minimum and maximum cell numbers for each material. Also sets indices for the last region with a cell turned on and the last cell turned on.

HEI

Calculates the total internal energy of a region of solid HE relative to the energy of its products at infinite expansion at T = 0.

GASLM

Finds limits for the region in which two of the analytic fits in GAS are reasonable.

BLDSM

Calculates the γ for each cell using the buildup model. The transition from constant γ_{max} to the $\gamma = A + B/R$ form is smoothed out with a parabola which joins both curves, leaving the first derivative continuous.

PRNT

Makes a cycle printout including time, Δt, cycle #, region and total energies, and cell quantities for active cells.

ESUM

Calculates kinetic, internal, and total energies for each region and for the whole problem.

WDUMP

Writes a restart dump (all of the necessary data to restart the problem at a given cycle). Inactive regions may be replaced with new setup information so that two different problems that start out the same may be restarted at a time before they differ without completely rerunning the problem.

RDUMP

Reads the restart dump and stores all of the data in the appropriate locations.

OUTGAS

Makes a GAS dump to file GASSIN which includes most cell quantities. GASSIN may be postprocessed to give on the Tektronix/film/fiche any cell variable as a function of any other cell variable (e.g., pressure vs radius) at a given time, time plot a cell variable for a given cell, r-t plots of interfaces, cell positions for each cell, contour plots of a cell variable in r-t space, etc.

ICONV

Takes a 60-bit floating point word and converts it to a 20-bit floating point word.

DIFEQ

Switching routine to determine the type of difference equation scheme to be used in the main hydro cycle. Default is HYDRO.

HYDRO

The main hydro cycle using the HYDROX difference equations. New values of radii, velocities, specific volumes, specific internal energies, and stress deviators are calculated. Subroutines are called to get new pressures, temperatures, and artificial viscosities.

SINX

The main hydro cycle using the SIN difference equations. New values of radii, velocities, specific volumes, specific internal energies, and stress deviators are calculated. Subroutines are called to get new pressures, temperatures, and artificial viscosities.

EOS

Switching routine to call the appropriate equation of state. The spalling and elastic-plastic treatments are also called if turned on.

PTEOS

Controls calls to EOS subroutines with energy and volume as input rather than region # and cell #.

HOM

Switching routine for deciding which type of EOS is used for a cell for the HOM EOS (e.g., determines whether a material is a solid, gas, or mixture).

USUP

USUP EOS allows for two USUP fits with a phase change. At high density the Barnes EOS is used. In tension, the Grüneisen EOS with the P=0 line as the standard curve is used.

GAS

Calculates the EOS for gases using analytic fits to the results of the BKW code. By special choice of constants, a γ-law gas EOS may be calculated.

SSBGAS

Calculates the pressure and specific internal energy for a cell that has just been burned using the sharp-shock burn method. The pressure and specific internal energy are calculated on the Hugoniot for the HE products at the given volume.

MIX

Calculates pressure and temperature for a mixture of solid and gas where temperature and pressure are assumed to be in equilibrium. The equations of state for the solid and gas are described more fully in USUP and GAS, respectively.

LFB

A two-point iteration scheme to find the zero of a function of one variable. The iteration is a slightly modified form of the secant method. This method is faster than Newton-Raphson iteration for the case where the time required to evaluate the derivative is longer than 0.44 of the time required to evaluate the function.

BEQST

The Barnes EOS is used for the high-pressure region where the USUP fit becomes unphysical.

BLDUP

Calculates the equation of state to be used with the buildup burn model. The EOS is that of a γ-law gas but the γ is not necessarily the same for all cells in a given material.

SPEOS

Determines whether a cell should spall by using the gradient spall model. As a special case, a constant spall pressure may be specified.

POLY

An eight-parameter fit to the equation of state that is basically a polynomial in two variables divided by a linear function in one of the variables. The two variables are related to specific volume and specific internal energy.

VISC

Computes the viscosity for all cells using either "real," PIC, or Landshoff-type viscosity.

BURN

Switching routine to determine type of burn to be used.

ARH

Calculates the decomposition due to an Arrhenius rate law for region I.

CJ

Calculates the decomposition of a detonating HE using the CJ burn model.

SSB

Calculates the decomposition of an HE using a sharp shock model. All of the HE is burned at the shock front.

FOREST

Calculates the decomposition using the Forest Fire burn model. This model is appropriate for cases that require a non-negligible distance of run to detonation for the given input shock strength.

FFT

The Forest Fire rate is calculated as a function of temperature.

FFI

The Forest Fire rate is calculated as a function of specific internal energy.

GLTW

An entire region of explosive is burned using the gamma-law Taylor-wave description.

BNDR1

Calculates several special boundary conditions such as an applied piston.

SL

Does all the bookkeeping required to create a spall.

SPLTCHK

Checks whether rezoning is required in a region and if so calls subroutines to do the rezoning.

SHFT

Shifts all cells with cell # $\geq$ J up by N. Used when new cells are created in the middle of the problem; e.g., for spall and rezoning.

SPLIT

Splits N cells starting at cell #J into two cells. All cell quantities are linearly interpolated and conservation of mass is explicitly required.

EPP

An elastic—perfectly plastic model with the von Mises yield model and an optional correction term to put shock data fit equations of state on the hydrostat.

DELT

Calculates the time step to be used. The time step may be input data or may be evaluated from several criteria in order to keep the problem numerically stable.

C

Switching function subroutine to pick the appropriate sound speed subroutine.

CUSUP

Calculates the sound speed for a USUP EOS with constant Grüneisen γ.

CBLDUP

Calculates the sound speed for a buildup EOS in cell J.

CPOLY

Calculates the sound speed at specific volume VC, pressure PC, and specific internal energy XC for the eight-parameter fit EOS in subroutine POLY.

CSES

Calculates the sound speed for a SESAME EOS.

RLEOS

The Rayleigh line in P-V space is used as an equation of state for the initial compression of the two cells touching an interface that has just become a closed void when the relative velocity of the two surfaces was large.

RL

Calculates parameters for the Rayleigh line EOS. This primarily consists of iteration to find the interface velocity which sends shock waves into both materials with the same final pressure.

G

Given a value for the interface particle velocity, UV, the difference in the corresponding Hugoniot pressures of the two bounding cells is calculated.

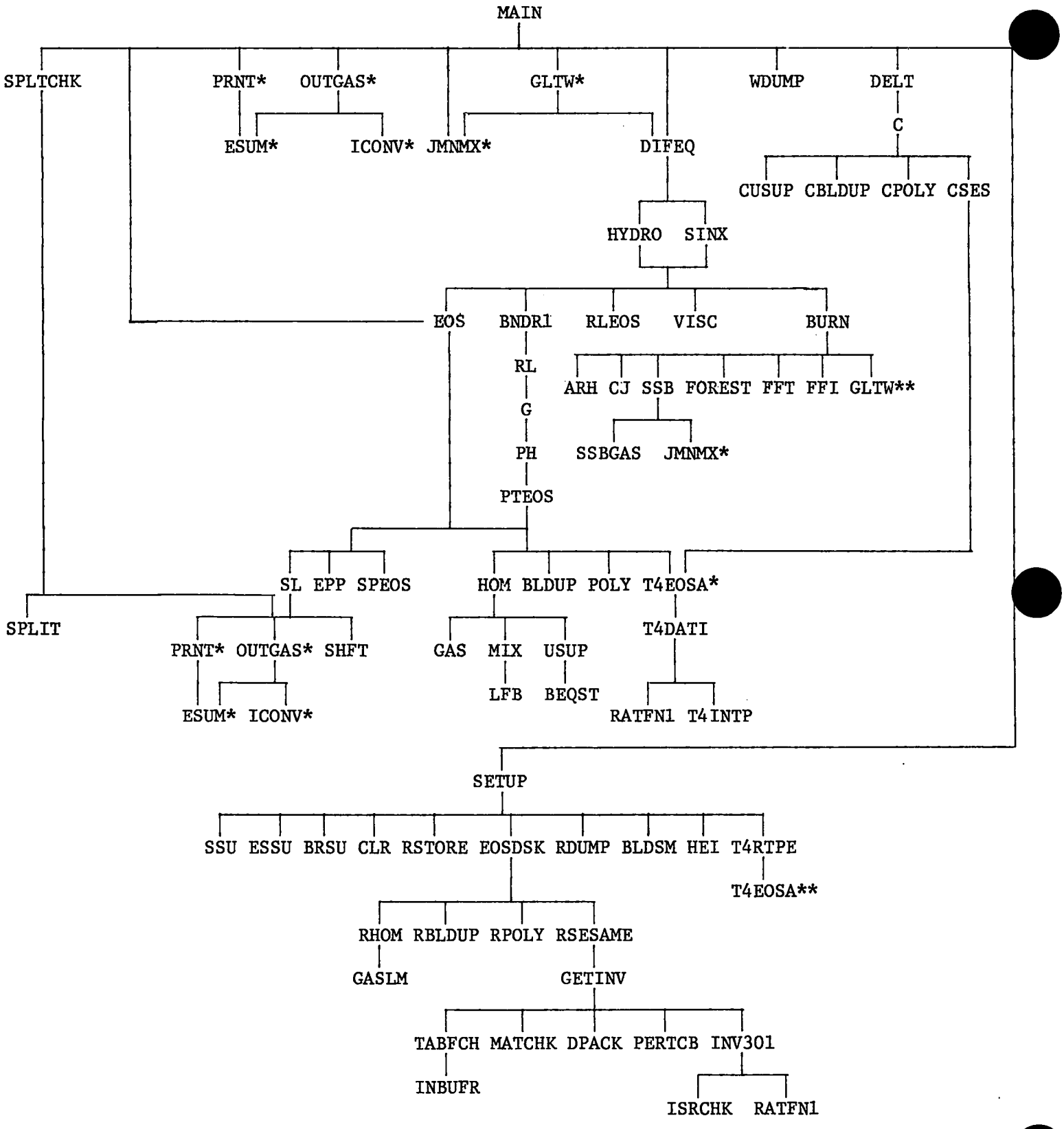
PH

For a given specific internal energy, the volume on the Hugoniot and the Hugoniot pressure are determined.

Subroutines Needed for the SESAME Tables

The following subroutines are used in conjunction with the SESAME EOS tables and are described in Sec. IV.E: MATCHK, TABFCH, INBUFR, DPACK, ISRCHK, T4INTP, GETINV, RATFN1, T4DATI, T4RTPE, INV301, T4EOSA, PERTCR.

B. Chart of the Relation Between Subroutines



*Subroutines that appear more than once.
**Subroutines that appear more than once and subroutines called by this subroutine are shown elsewhere on the chart.

C. Variables in Common Blocks Not Already Described

/CELL/

R = outside radius of a cell (cm).

U = velocity (cm/μs).

V = specific volume = $1/\rho$ ($cm^3 g$).

XI = specific internal energy (Mbar-cm^3/g).

P = pressure (Mbar).

SX = stress deviator in the X-direction (Mbar).

SZ = stress deviator in the Z-direction (Mbar).

EE = energy sums, see ESUM.

T = temperature (K) or γ for Buildup EOS.

Q = artificial viscosity (Mbar).

XM = mass in grams per unit length or solid angle.

IFLAG = flags associated with a cell.

W = mass fraction of undecomposed explosive (i.e., W = 1 for all solid, W = 0 for all gas).

/OVL/ See INP namelist.

/MISC/

TIME = time (μs).

ICYCL = cycle #.

DT = time step (μs).

NCL = last cell # + 1.

IA = IALPH - 1.

BU = current outside piston velocity (cm/μs).

BUI = current inside piston velocity (cm/μs).

F2,F3 = geometry-dependent coefficients used in the calculation of the specific volume of a cell.

/BRNS/ See BEQST for details.

A = A.

BR = b_r.

BA = b_a.

VBO = V_0.

VBSW = volume below which BEQST is used instead of USUP.

/EOSN/ See SU namelist.

/NSPLT/ See SU namelist.

/SPC/ See ESC namelist.

/POLYC/ See ESC namelist.

/GAS/ See OUTGAS for details.

FI = index for GAS dumps.

DI = array for all cell variables (equivalenced to R).

/LEV/

DMPNO = dump # = time (see OUTGAS).

/BUX/ See ESC namelist.

/ES/ See ESC namelist.

/RLC/ See RLEOS, RL, G, and PH for details.

RC = R_c.

RP = R_p.

RLV = R_ℓ.

PH1 = $P_H^{(1)}$

DV1 = ΔV_1

DV2 = ΔV_2

/PWORK/ See BNDR1, ESUM.

PW = work done by the outside piston (if used).

PWI = work done by the inside piston (if used).

JS = spall indicator. Whenever JS $\neq$ 0, a new void is created at the outside radius of cell JS.

/INIT/ See SU, ESC namelists.

JMIN = minimum cell # for this region.

JMAX = maximum active cell # for this region.

DR0 = initial Δr for the innermost cell of the region.

/USUPC/ See ESC namelist.

/BRND/ See BURN namelist.

/GASC/ See ESC namelist.

/FGHIJC/ See ESC namelist.

/UCJC/

UCJ = CJ velocity.

JJ = cell # being burned in SSB.

NMAX = last cell currently active.

RCJ = radius of the cell being burned in SSB.

DCJ = CJ detonation velocity.

/VOID/

INTX = type of interface: $1(\mu_I = \mu_{I+1} = 0)$, $2(\mu_I = 0, \mu_{I+1} \neq 0)$, $3(\mu_I \neq 0, \mu_{I+1} = 0)$, $4(\mu_I \neq \mu_{I+1} \neq 0)$, $5(\mu_I = \mu_{I+1} \neq 0)$.

JV = cell # of the artificial cell used to describe a void between region I and I + 1.

IV = see SU namelist.

NNV = # of voids.

/MNMX/

KMAX = maximum cell # for a region.

KMIN = minimum cell # for a region.

NMC = # of regions currently active.

/XCOM/ See SU, ESC namelists.

/INTORD/ See INP namelist.

/EOSCOM/ See ESC namelist.

/XEOS/

IX = region #.

/SESDAT/

DC = array for SESAME tables.

/S2DIR/

LCMX = # of words in DC.

NREG = # of regions allowed.

LCFW = word # in DC that begins data for region I.

/SESIN/

II = region #.

IDT = data type.

RPT4 = density.

XIPT4 = specific internal energy.

IBR = 0 to output P and T; 1 to output P; 2 to output T.

IFL = 0 allows for a ramp; 1 requires use of tables.

/SESOUT/

PPT4 = P, $\partial P/\partial \rho$, $\partial P/\partial E$.

TPT4 = T, $\partial T/\partial \rho$, $\partial T/\partial E$.

D. Annotated Subroutine Listings and Detailed Notes

```
      PROGRAM HYDROX(INPUT,OUTPUT,DATA,TAPE5=DATA,DOUT,TAPE6=DOUT,        MAIN      2
     +XOUT,TAPE8=XOUT,TTY,TAPE9=TTY)                                      MAIN      3
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,           PARAM     2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                    PARAM     3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                      PARAM     4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                          PARAM     5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                           MCELL     2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)     MCELL     3
     +,W(MCL)                                                             MCELL     4
      LEVEL 2,R                                                           MCELL     5
      COMMON/DVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UTI,UFI,NADD,NM,   MCELL     6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                      MCELL     7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                    MCELL     8
      LEVEL 2,TIME                                                        MCELL     9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),°O   INIT      2
     +(ML),TO(ML),RDW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML),  INIT      3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)              INIT      4
      COMMON/USUPC/C1(ML),S1(ML),C2(ML),S2(ML),SWV(ML),VMN(ML),           US        2
     +GAMMA(ML),ALP(ML)                                                   US        3
      COMMON/BRND/Z(ML),E(ML),VCJ(ML),DWDT(NDW,ML),PCJ(ML),PM(ML),ND(ML)  BRD       2
     +,MSFF                                                               BRD       3
      COMMON/GASC/GC(NGC,ML)                                              GC        2
      COMMON/FGHTJC/FS(ML),GS(ML),HS(ML),SI(ML),SJ(ML),CV(ML)             FG        2
      COMMON/UCJC/UCJ,JJ,NMAX,RCJ,DCJ                                     UC        2
      COMMON/VOID/INTX(ML2),JV(ML2),IV(ML2),NNV                           VD        2
      COMMON/MNMX/KMAX(ML2),KMIN(ML2),NMC                                 MN        2
      COMMON/BRNS/A(ML),BR(ML),BA(ML),VBO(ML),VBSW(ML)                    BRN       2
      COMMON/EOSN/IEOS(ML),ME(ML)                                         EN        2
      COMMON/NSPLT/NOSPLT(ML2)                                            NSP       2
      COMMON/SPC/SP(ML),USP(ML)                                           SPLC      2
     +,XISP(ML)                                                           SPLC      3
      COMMON/POLYC/CF(NCF,ML),PS(ML)                                      PLC       2
      COMMON/GAS/FI(1003),DI(MQL)                                         GS        2
      LEVEL 2,FI                                                          GS        3
      COMMON/LEV/DMPNO                                                    GS        4
      LEVEL 2,DMPNO                                                       GS        5
      COMMON/BUX/BUA,BUB,BUMAX,BUDV(ML)                                   BUP       2
     +,BUR,BUD                                                            BUP       3
      COMMON/ES/TE(ML2),NME                                               ESM       2
      COMMON/RLC/RC(ML),RP(ML),RLV(ML),PH1,DV1,DV2                        RLC       2
      COMMON/PWORK/PW,PWI                                                 PWORK     2
      TIME=0.  Start at t = 0                                             MAIN     24
      CALL SETUP  Set up the problem                                      MAIN     25
      ISS=0                                                               MAIN     26
      DO 8 I=1,NM                                                         MAIN     27
      IF(IBRN(I).NE.3)GO TO 8   Initialization for sharp-shock burn only  MAIN     28
      IF(ISS.NE.0)GO TO 8                                                 MAIN     29
      JJ=JMIN(I)                                                          MAIN     30
      ISS=I                                                               MAIN     31
      NMAX=JJ                                                             MAIN     32
    8 CONTINUE                                                            MAIN     33
      CALL JMNMX(NMAX)  Initialize indices for min. and max. cell # in each region  MAIN  34
      IF(IDMP.NE.0)GO TO 10  Skip to 10 if a restart                      MAIN     35
      NMCT=NMC                                                            MAIN     36
      NMC=NM                                                              MAIN     37
      JMT=JMAX(NMCT)                                                      MAIN     38
      JMAX(NMCT)=KMAX(NMCT)                                               MAIN     39
      RCJ=0.                                                              MAIN     40
      DO 9 I=1,NM                                                         MAIN     41
      IF(IBRN(I).EQ.7)CALL GLTW(I)  Do any gamma-law Taylor wave first    MAIN     42
```

```
      IF(RCJ.NE.0..OR.IBRN(I).NE.3)GO TO 9   ]                          MAIN      43
      RCJ=R(JJ)                              ]                          MAIN      44
      IF(I.EQ.1)GO TO 9                      ]  More setup for          MAIN      45
      DCJ=VCJ(I)                             ]   sharp shock burn       MAIN      46
      DT=(R(JJ)-R(JJ+1))/(DCJ*4)             ]                          MAIN      47
      UCJ=-E(I)                              ]                          MAIN      48
    9 CONTINUE                                                           MAIN      49
      CALL EOS  Initialize P,T for all cells                             MAIN      50
      JMAX(NMCT)=JMT                                                     MAIN      51
      NMC=NMCT                                                           MAIN      52
   10 CONTINUE                                                           MAIN      53
      MG=0                                   ]                          MAIN      54
      TMP=TP(1)                              ]                          MAIN      55
      TMG=TG(1)                              ]                          MAIN      56
      TPMX=TMP                               ]                          MAIN      57
      TGMX=TMG                               ]  Setup for print, gas dump, restart dump   MAIN      58
      ITP=0                                  ]  Keyed to certain cycle #'s and times      MAIN      59
      ITG=0                                  ]                          MAIN      60
      TMD=TD(1)                              ]                          MAIN      61
      TDMX=TMD                               ]                          MAIN      62
      ITD=0                                  ]                          MAIN      63
      MP=0                                   ]                          MAIN      64
      MD=0                                   ]                          MAIN      65
      ICYCL=0                                                            MAIN      66
      CALL PRNT   Printout of initial conditions                         MAIN      67
      BU=UI                                  ]                          MAIN      68
      BUI=UII                                ]  Initial piston velocities and work        MAIN      69
      PW=0.                                  ]                          MAIN      70
      PWI=0.                                 ]                          MAIN      71
      CALL GASSIGN(3,6HGASSIN,0,0)  GASSIN = file for GAS dumps          MAIN      72
      IF(NADD.LE.0)NADD=5                                                MAIN      73
      CALL OUTGAS  GAS dump of initial conditions                        MAIN      74
      DO 20 II=1,NI   Main do loop of the code.  NI is the maximum # of cycles     MAIN      75
      ICYCL=II                                                  allowed  MAIN      76
      MP=MP+1                                                            MAIN      77
      MG=MG+1                                                            MAIN      78
      MD=MD+1                                                            MAIN      79
      IF(IBRN(NMC).EQ.3)GO TO 123  Except for sharp-shock burn           MAIN      80
      IF(NMAX.EQ.NCL-1)GO TO 123    or for all cells active              MAIN      81
      JMC=JMAX(NMC)                                  Check to see if the last    MAIN      82
      IF(ABS(U(JMC)-UO(NMC)).LT.UT(NMC))GO TO 123   active cell is moving MAIN      83
      NMAX=NMAX+NADD                         ]                          MAIN      84
      IF(NMAX.GT.NCL-1)NMAX=NCL-1            ]  If so, add NADD         MAIN      85
      CALL JMNMX(NMAX)                       ]  New active cells        MAIN      86
  123 CONTINUE                                                           MAIN      87
      CALL SPLTCHK  Check for rezoning                                   MAIN      88
      CALL DELT   Check time step                                        MAIN      89
      TIME=TIME+DT   Increment time step                                 MAIN      90
      IF(W(3).LT.0.02) BU=UF                 ]  Use final piston velocity when the      MAIN      91
      IF(W(NCL-3).LT.0.02)BUI=UFI            ]   3rd cell in has burned MAIN      92
      CALL DIFEQ   Main hydro done here                                  MAIN      93
      IF(NP.LE.0)GO TO 15                    ]                          MAIN      94
      IF(MP.LT.NP)GO TO 15                   ]  Check for print every NP cycles           MAIN      95
      MP=0                                   ]                          MAIN      96
      CALL PRNT                              ]                          MAIN      97
   15 CONTINUE                                                           MAIN      98
      IF(NG.LE.0)GO TO 16                    ]                          MAIN      99
      IF(MG.LT.NG)GO TO 16                   ]  Check for GAS dump every NG cycles        MAIN     100
      MG=0                                   ]                          MAIN     101
      CALL OUTGAS                            ]                          MAIN     102
```

```
 16 CONTINUE                                                              MAIN      103
    IF(TP(2).LE.0.)GO TO 17                                               MAIN      104
    IF(TIME.LT.TMP)GO TO 17                                               MAIN      105
    TMP=TMP+TP(2)                                                         MAIN      106
    IF(TMP.LT.TPMX)GO TO 27                                               MAIN      107
    TMP=TPMX                  Check for print on time interval            MAIN      108
    ITP=ITP+2                                                             MAIN      109
    TP(2)=TP(ITP)                                                         MAIN      110
    TPMX=TP(ITP+1)                                                        MAIN      111
 27 CALL PRNT                                                             MAIN      112
 17 CONTINUE                                                              MAIN      113
    IF(TG(2).LE.0.)GO TO 18                                               MAIN      114
    IF(TIME.LT.TMG)GO TO 18                                               MAIN      115
    TMG=TMG+TG(2)                                                         MAIN      116
    IF(TMG.LT.TGMX)GO TO 28                                               MAIN      117
    TMG=TGMX                  Check for GAS dump on time interval         MAIN      118
    ITG=ITG+2                                                             MAIN      119
    TG(2)=TG(ITG)                                                         MAIN      120
    TGMX=TG(ITG+1)                                                        MAIN      121
 28 CALL OUTGAS                                                           MAIN      122
 18 CONTINUE                                                              MAIN      123
    IF(NDUMP.EQ.0)GO TO 19                                                MAIN      124
    IF(MD.LT.NDUMP)GO TO 19   Check for restart dump every ND cycles      MAIN      125
    MD=0                                                                  MAIN      126
    CALL WDUMP                                                            MAIN      127
 19 CONTINUE                                                              MAIN      128
    IF(TD(2).LE.0.)GO TO 29                                               MAIN      129
    IF(TIME.LT.TMD)GO TO 29                                               MAIN      130
    TMD=TMD+TD(2)                                                         MAIN      131
    IF(TMD.LT.TDMX)GO TO 39                                               MAIN      132
    TMD=TDMX                  Check for restart dump on time interval     MAIN      133
    ITD=ITD+2                                                             MAIN      134
    TD(2)=TD(ITD)                                                         MAIN      135
    TDMX=TD(ITD+1)                                                        MAIN      136
 39 CALL WDUMP                                                            MAIN      137
 29 CONTINUE                                                              MAIN      138
    IF(TIME.GE.TEND.AND.TEND.GT.0.)GO TO 999   Stop for t > TEND ≠ 0      MAIN      139
 20 CONTINUE                                                              MAIN      140
999 CONTINUE                                                              MAIN      141
    CALL WDUMP                                                            MAIN      142
    CALL PRNT     Make a last restart dump and print                      MAIN      143
    STOP                                                                  MAIN      144
    END                                                                   MAIN      145
```

Calls routines to set up the problem.

Contains the main cycle loop of the code which checks whether to add cells, print, make a GAS dump, make a restart dump, or end the problem; calls subroutines to rezone if necessary, determine the time step, and run one hydro cycle.

Local Variables

MP,MG,MD = # of cycles since the last print, GAS dump, restart dump.

TMP,TMG,TMD = time at which the next print, GAS dump, restart dump will be made.

ITP,ITG,ITD = index for which t,Δt to use.

TPMX,TGMX,TDMX = time at which a switch is made to the next Δt.

II = cycle #, do loop count.

JMC = JMAX(NMC) is the last cell currently turned on.

JMT = temporary storage of JMAX(NMC) so that it can be changed for the call to EOS.

NMCT = temporary storage of NMC.

Notes

The sharp-shock burn uses its own method for adding a cell every four cycles as the shock goes through the material (see SSB).

The algorithm for printing, etc., every N dumps is: initialize an index M to 0, increment by 1 each cycle. When M = N print, etc. and reset M to 0.

The algorithm for printing, etc., on $t_1,\Delta t_1,\cdots$ is: initialize a parameter T to t_1. When the time is $\geqslant$ T print, etc. Reset T to T + Δt_1 unless T + $\Delta t_1 > t_2$. Then set T to t_2 and increment by Δt_2, etc.

The common blocks should be all kept in MAIN even though they are not all used. This is due to the fact that the restart dumps are keyed on the first

location in one common block and the last location in a different common block. The order in which the common blocks are stored is, therefore, important. By including all the common blocks required for a restart dump in MAIN, their order in storage will be that required by WDUMP and RDUMP (q.v.).

```
      SUBROUTINE SETUP                                                  SETUP     2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM     2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM     3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM     4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                        PARAM     5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                         MCELL     2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)   MCELL     3
     +,W(MCL)                                                           MCELL     4
      LEVEL 2,R                                                         MCELL     5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM, MCELL     6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                    MCELL     7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                  MCELL     8
      LEVEL 2,TIME                                                      MCELL     9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO  INIT      2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT      3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)            INIT      4
      COMMON/USUPC/C1(ML),S1(ML),C2(ML),S2(ML),SWV(ML),VMN(ML),         US        2
     +GAMMA(ML),ALP(ML)                                                 US        3
      COMMON/BRND/Z(ML),E(ML),VCJ(ML),DWDT(NDW,ML),PCJ(ML),PM(ML),ND(ML) BRD      2
     +,MSFF                                                             BRD       3
      COMMON/GASC/GC(NGC,ML)                                            GC        2
      COMMON/FGHIJC/FS(ML),GS(ML),HS(ML),SI(ML),SJ(ML),CV(ML)           FG        2
      COMMON/UCJC/UCJ,JJ,NMAX,RCJ,DCJ                                   UC        2
      COMMON/VOID/INTX(ML2),JV(ML2),IV(ML2),NNV                         VD        2
      COMMON/MNMX/KMAX(ML2),KMIN(ML2),NMC                               MN        2
      COMMON/BRNS/A(ML),BR(ML),BA(ML),VBO(ML),VBSW(ML)                  BRN       2
      COMMON/EOSN/IEOS(ML),ME(ML)                                       EN        2
      COMMON/NSPLT/NOSPLT(ML2)                                          NSP       2
      COMMON/SPC/SP(ML),USP(ML)                                         SPLC      2
     +,XISP(ML)                                                         SPLC      3
      COMMON/POLYC/CF(NCF,ML),PS(ML)                                    PLC       2
      COMMON/BUX/BUA,BUB,BUMAX,BUDV(ML)                                 BUP       2
     +,BUR,BUD                                                          BUP       3
      COMMON/ES/IE(ML2),NME                                             ESM       2
      LEVEL 2,DC                                                        LCMC      2
      COMMON/LCMC/DC(NSD)                                               LCMC      3
      COMMON/XCOM/R1,R2,DR1,DR2,WO,NCI,DR,ZI                            XC        2
      COMMON/INTORD/IFN                                                 SETUP    24
      COMMON/EOSCOM/SR(ML),ES(ML),A1(ML),A2(ML),A3(ML),EM(ML),IRV(ML)   EOSCOM    2
      NAMELIST/SU/DTO,NOSPLT,IV,IEOS,MAT,ME,R1,R2,UO,NCI                NMLST     2
     +,DR1,DR2,UT,DTCF,IJK                                              NMLST     3
      NAMELIST/ESC/C1,S1,C2,S2,SWV,VMN,GAMMA,ALP,A,BR,BA,VBO,VBSW,      NMLST     4
     +FS,GS,HS,SI,SJ,CV,GC,SP,USP,CF,PS,BUA,BUB,BUMAX,BUDV,TMLT,TMC,    NMLST     5
     +XMU,YO,XL,XV,VO,PO,TO,ROW,PLAP,IBRN,NV,WO,ZI                      NMLST     6
     +,SR,ES,A1,A2,A3,EM,IRV,BUR,BUD,XISP,QO,IE                         NMLST     7
      NAMELIST/BURN/Z,E,VCJ,PCJ,DWDT,PM,ND                              NMLST     8
      NAMELIST/INP/NM,UI,UF,RO,IALPH,NDF,NI,NP,NG,NADD,NMAX,            NMLST     9
     +TEND,TP,TG,NDELT,UII,UFI,LABEL,NM1,IDMP,IV,NDUMP,TD,IFN           NMLST    10
     +,NO,DTCF                                                          SETUP    29
     +,MSFF                                                             SETUP    30
      DATA NM1/1/,IDMP/0/,NNV/0/,NDUMP/10000/,TD/ML*0./                 SETUP    31
      DATA NM,UI,UF,RO,IALPH,NDF,NI,NP,NG,NADD,NMAX,TEND,TP,TG          SETUP    32
     +,UII,UFI,LABEL/0,3*0.,3,1,10000,4*0,0.,ML*0.,ML*0.,2*0.,          SETUP    33
     +8*10H          /                                                  SETUP    34
      DATA DTO,XMU,YO,XL,XV,VO,PO,TO,ROW,PLAP,IBRN,NV,NOSPLT,IV         SETUP    35
     +,UO,QO,TMLT,TMC                                                   SETUP    36
     +/ML*1.,ML*0.,ML*0.,ML*0.,ML*2.,ML*0.,ML*1.E-10,ML*0.,            SETUP    37
     +ML*0.,ML*0.,ML*0,ML*1,ML2*0,ML2*-1,ML*0.,ML*1.E-10,ML*0.,ML*0./  SETUP    38
      DATA R1,R2,WO,ZI,NCI/2*0.,1.,0.,0/                                SETUP    39
      DATA A,BR,BA,VBO,VBSW/ML*0.,ML*0.,ML*0.,ML*0.,ML*0./              SETUP    40
```

```
      DATA IEOS,MAT,ME/ML*1,ML*0,ML*0/                                  SETUP     41
      DATA C1,S1,C2,S2,SWV,VMN,GAMMA,ALP/ML*0,ML*0,ML*0,ML*0,ML*0,      SETUP     42
     +ML*0,ML*0,ML*0/                                                   SETUP     43
      DATA Z,E,VCJ,PCJ,PM,ND/ML*0,ML*0,ML*0,ML*0,ML*0,ML*0/             SETUP     44
      DATA FS,GS,HS,SI,SJ,CV/ML*0.,ML*0.,ML*0.,ML*0.,ML*0.,ML*0./       SETUP     45
      DATA SP,USP/ML*0.,ML*0./                                          SETUP     46
      DATA GC/MLGC*0/                                                   SETUP     47
      DATA DWDT/MLDWDT*0/                                               SETUP     48
      DATA IFN/0/                                                       SETUP     49
      DATA SR,ES,A1,A2,A3,EM,IRV/ML*1.,ML*0.,ML*0.,ML*0.,ML*0.,ML*1000. SETUP     50
     +,ML*0/                                                            SETUP     51
      DATA UT/ML*1.E-10/,NO/180/,DTCF/ML*0.5/                           SETUP     52
      DATA MSFF/0/                                                      SETUP     53
      DATA XISP/ML*0./                                                  SETUP     54
      DATA BUD/.2/                                                      SETUP     55
      READ(5,INP)   Read INP namelist                                   SETUP     56
      IF(IDMP.EQ.0)GO TO 99   Check whether to use a restart dump       SETUP     57
      CALL RDUMP(IDMP)  Read 1st dump after cycle IDMP                  SETUP     58
      READ(5,INP)  Make any necessary changes in INP variables          SETUP     59
      IF(NM1.EQ.1)RETURN   If no new materials are added, setup is complete SETUP 60
   99 CONTINUE                                                          SETUP     61
      DO 1 I=NM1,NM                                                     SETUP     62
    1 IE(I)=I                                                           SETUP     63
      SRDR=RO/NO  Default value used in automatic zoning                SETUP     64
      R1=RO  Default value for R1                                       SETUP     65
      IA=IALPH-1                                                        SETUP     66
      J=1   J = cell #                                                  SETUP     67
      IF(IDMP.NE.0)J=KMAX(NM1-1)  For a restart with new materials added, do SETUP 68
      F2=0.5                       setup only for the new materials     SETUP     69
      F3=0.                                                             SETUP     70
      IF(IA.NE.2)GO TO 15  Geometry factors                             SETUP     71
      F2=1./3.                                                          SETUP     72
      F3=1.                                                             SETUP     73
   15 CONTINUE                                                          SETUP     74
      IF(IDMP.EQ.0)R(1)=RO  Set piston radius to RO unless a restart    SETUP     75
      DO 10 I=NM1,NM                                                    SETUP     76
      CALL CLR   Set default values for region 1                        SETUP     77
      CALL SSU(I)  Read SU namelist                                     SETUP     78
      IF(MAT(I+1).NE.0) CALL EOSDSK(I)  For MAT ≠ 0 read EOS data from disk SETUP 79
      IF(ME(I+1).EQ.0.AND.MAT(I+1).NE.0) GO TO 30  More data?           SETUP     80
      CALL ESSU(I)  Read ESC namelist                                   SETUP     81
   20 IF(IBRN(I+1).EQ.0) GO TO 30                                       SETUP     82
      CALL BRSU(I)  Read BURN namelist                                  SETUP     83
   30 R(J+1)=R1  Outside radius for region I                            SETUP     84
      IF(ZI.NE.0.)GO TO 50                                              SETUP     86
      IF(TO(I+1).EQ.0..OR.IEOS(I+1).NE.4)GO TO 50  Calculate I0 for     SETUP     87
      II=I+1                                        input T0 in SESAME  SETUP     88
      CALL T4RTPE(I,1,DC,ROW(II),TO(II),PP,ZI,IFL)                      SETUP     89
   50 CONTINUE                                                          SETUP     90
      IFL=64*I  Region # flag                                           SETUP     92
      IF(DTO(I+1).LE.0..OR.DTO(I+1).EQ.1.)DTO(I+1)=DTO(2)               SETUP     93
      IF(DTCF(I+1).LE.0..OR.DTCF(I+1).EQ.0.5)DTCF(I+1)=DTCF(2)          SETUP     94
      U(J+1)=UO(I+1)  Initial velocity for the region                   SETUP     95
      JMIN(I)=J+1                                                       SETUP     96
      DS=0.                                                             SETUP     97
      IF(NCI.NE.0.)GO TO 12                                             SETUP     98
      IF(DR1.LE.0.)GO TO 14                                             SETUP     99
      NCI=2*(R1-R2)/(DR1+DR2)                                           SETUP    100
      DS=2*(R1-R2-NCI*DR1)/(NCI*(NCI-1))  Variable zone size            SETUP    101
      DR=DR1                                                            SETUP    102
```

```
      DRO(I+1)=DR2                                                      SETUP    103
      GO TO 13                                                          SETUP    104
   14 CONTINUE                                                          SETUP    105
      DR=SRDR/SQRT(ROW(I+1))                                            SETUP    106
      NCI=(R1-R2)/DR+0.5                                                SETUP    107
      IF(NCI.LT.4)NCI=4                          Automatic zoning       SETUP    108
      IF(NCI.GT.NO/4.AND.ROW(I+1).GT.10.)NCI=NO/4                       SETUP    109
      IF(NCI.LT.8.AND.ROW(I+1).GT.5.)NCI=8                              SETUP    110
   12 CONTINUE                                                          SETUP    111
      DR=(R1-R2)/NCI   NCI equally sized zones                          SETUP    112
      DRO(I+1)=DR                                                       SETUP    113
   13 CONTINUE                                                          SETUP    114
      DO 11 K=1,NCI  Initialize cell quantities in this region          SETUP    115
      J=J+1                                                             SETUP    116
      W(J)=WO  Burn fraction                                            SETUP    117
      T(J)=TO(I+1)  Temperature                                         SETUP    118
      XI(J)=ZI  Specific internal energy                                SETUP    119
      R2=R1-DR                                                          SETUP    120
      XM(J)=F2*DR*(R1**IA+R2**IA+F3*R1*R2)*ROW(I+1) Mass/unit solid angle or area SETUP 121
      V(J)=F2*DR*(R1**IA+R2**IA+F3*R1*R2)/XM(J)  Specific volume        SETUP    122
      R1=R2                                                             SETUP    123
      R(J+1)=R1  Outside radius of the cell                             SETUP    124
      IFLAG(J)=IFL                                                      SETUP    125
      U(J+1)=UO(I+1)  Velocity                                          SETUP    126
      DR=DR+DS  For variable zone size                                  SETUP    127
11    CONTINUE                                                          SETUP    128
      JMAX(I)=J  Maximum cell # in the region                           SETUP    129
C BUILD UP EOS CONSTANTS                                                SETUP    130
      IF(IEOS(I+1).NE.2) GO TO 40                                       SETUP    131
      JMN=JMIN(I)                                                       SETUP    132
      JMX=JMAX(I)                                                       SETUP    133
      BUDV(I+1)=BUDV(I+1)**2          For Buildup EOS calculate γ for each SETUP 134
      DO 41 K=JMN,JMX                  cell and store in temperature    SETUP    135
      DR=R(JMN)-(R(K+1)+R(K))/2+BUR                                     SETUP    136
      T(K)=BLDSM(DR,I)                                                  SETUP    137
   41 CONTINUE                                                          SETUP    138
   40 CONTINUE                                                          SETUP    139
      VO(I+1)=V(J)  Initial specific volume for the region              SETUP    140
      IF(IBRN(I+1).NE.0)CALL HEI(I+1)  Shift in energy zero for HE's    SETUP    141
      IF(IV(I+1).LT.0)GO TO 10                                          SETUP    142
      J=J+1                                                             SETUP    143
      NNV=NNV+1   Set up the artificial cell used for voids             SETUP    144
      XM(J)=0.                                                          SETUP    145
      JV(I)=J                                                           SETUP    146
10    CONTINUE                                                          SETUP    147
      CALL RSTORE  All region quantities shifted down one to their proper places SETUP 148
      NMM=NM-1                                                          SETUP    149
      DO 180 I=1,NMM                                                    SETUP    150
      I1=1                                                              SETUP    151
      I2=1                                                              SETUP    152
      IF(XMU(I).EQ.0.) I2=0          Set up flags for the type          SETUP    153
      IF(XMU(I+1).EQ.0.)I1=0          of interface (see HYDRO)          SETUP    154
      II=I2*2+I1+1                                                      SETUP    155
      IF(II.EQ.4.AND.XMU(I).EQ.XMU(I+1))II=5                            SETUP    156
      INTX(I)=II                                                        SETUP    157
  180 CONTINUE                                                          SETUP    158
      INTX(NM)=1                                                        SETUP    159
      IF(XMU(NM).NE. 0.) INTX(NM)=3  Interface flag for inside free surface SETUP 160
      NCL=J+1                                                           SETUP    161
      R(NCL+1)=R(NCL)                                                   SETUP    162
```

```
      IFLAG(NCL)=IFLAG(NCL-1)+64                                        SETUP     163
      DT=DTO(1)                                                         SETUP     164
      IF(NADD.LE.0)NMAX=NCL-1    for NADD ≤ 0, start with all cells active SETUP     165
      DO 200 I=1,NM                                                     SETUP     166
      SROW=SQRT(ROW(I))                                                 SETUP     167
      JMN=JMIN(I)                                                       SETUP     168
      JMX=JMAX(I)                                                       SETUP     169
      J=JMX-JMN+1                                                       SETUP     17C
      SR1=(R(JMN)-R(JMN+1))*SROW                                        SETUP     171
      SR2=(R(JMX)-R(JMX+1))*SROW                                        SETUP     172
      PRINT 201,T,J,IEOS(I),MAT(I),SR1,SR2                              SETUP     173
  201 FORMAT(4I5,2(1PE10.3))                                            SETUP     174
  200 CONTINUE                                                          SETUP     175
      IF(UI.NE.0..OR.IEOS(1).NE.2)GO TO 211                             SETUP     176
      UI=-SQRT(BUOV(1))/(T(2)+1)  Automatic setup of piston velocities for SETUP  177
      UF=-UI*.8                    Buildup EOS                          SETUP     178
  211 CONTINUE                                                          SETUP     179
      IF(IBRN(1).NE.3.OR.IDMP.NE.0)GO TO 210                            SETUP     180
      DCJ=VCJ(1)                                                        SETUP     181
      IF(IEOS(1).EQ.2)DCJ=SQRT(BUOV(1))                                 SETUP     182
      DT=(R(2)-R(3))/(DCJ*4)                                            SETUP     183
      UCJ=UI                       Setup for sharp shock burn           SETUP     184
      IF(E(1).LE.0.)GO TO 210                                           SETUP     185
      UI=-E(1)                                                          SETUP     186
      UF=E(1)*0.8                                                       SETUP     187
      UCJ=UI                                                            SETUP     188
  210 CONTINUE                                                          SETUP     189
      WRITE(6,INP)                                                      SETUP     190
      WRITE(6,SU)                                                       SETUP     191
      WRITE(6,ESC)  Write out all of the namelist variables on DOUT     SETUP     192
      WRITE(6,BURN)                                                     SETUP     193
      CALL CLOSE(6)                                                     SETUP     194
      RETURN                                                            SETUP     195
      END                                                               SETUP     196
```

SETUP

Controls the setup of the problem, reads INP namelist, checks for a restart dump, calls other routines to read the rest of the namelists data from EOS files, initializes all of the cell quantities except pressure, writes out all variables in all namelists to the file DOUT.

Local Variables

SRDR = RO/NO = the value of $\sqrt{\rho_0}\,\Delta r$ to be used in automatic zoning. It is set such that approximately NO cells would be used in the problem if ρ_0 were 1.0 for each material and the innermost cell of the problem were at r = 0.

J = cell # index.

RD = outside radius of the problem.

I = region # index.

PP = pressure from SESAME for input ρ_0, T_0.

IFL = flag = 1 for success = 0 for failure to find P,I for input ρ_0, T_0; also the region number flag in IFLAG used in OUTGAS.

DS = the change in Δr per cell if a linearly varying Δr is used.

K = kth cell in a region or cell # index.

NMM = NM-1.

I1= 0 if $\mu_I = 0$, 1 if $\mu_I \neq 0$.

I2 = 0 if $\mu_{I+1} = 0$, 1 if $\mu_{I+1} \neq 0$.

II = temporary variable in which INTX is computed; also I + 1.

SROW = $\sqrt{\rho_0}$.

SR1 = $\sqrt{\rho_0}\,\Delta r$ for the outermost cell of the region.

SR2 = $\sqrt{\rho_0}\,\Delta r$ for the innermost cell of the region.

JMN,JMX = JMIN(I),JMAX(I).

Notes

The zoning in a region may be set up such that the cell size varies linearly with cell number; that is,

$$\Delta r_n = \Delta r^{(1)} + S(n - 1) \quad , \tag{1}$$

where n is the number of the cell counting inward from the first cell in the region, $\Delta r^{(1)}$ is Δr_1, and S is a constant to be determined. The total distance spanned by N cells for given S is

$$r_1 - r_2 = \sum_{i=1}^{N} \Delta r_i = N\Delta r^{(1)} + S \frac{N(N - 1)}{2} \quad , \tag{2}$$

where r_1 is the outside radius of the region and r_2 is the inside radius. The cell size of the innermost cell is

$$\Delta r^{(2)} = \Delta r_N = \Delta r^{(1)} + S(N - 1) \quad . \tag{3}$$

The usual input quantities are r_1, r_2, $\Delta r^{(1)}$, and $\Delta r^{(2)}$. Using this information we can express S and N as

$$S = \frac{2\left(r_1 - r_2 - N\, r^{(1)}\right)}{N(N - 1)} \quad , \tag{4}$$

$$N = \frac{2(r_1 - r_2)}{\Delta r^{(1)} + \Delta r^{(2)}} \quad . \tag{5}$$

Note, however, that N will not be an integer for arbitrary input values. In order to avoid this problem, we take N as the integer part of the value given by Eq. (5). Then Eq. (4) is evaluated using the new integer value of N. The value of $\Delta r^{(2)}$ will then be slightly different from the input value.

The mass and volume calculations are the same as in HYDRO (q.v.). For Buildup EOS (see BLDUP), the value of γ for each cell is stored in the temperature, T. BUDV is input as the detonation velocity D, but it is stored in the code as D^2 to avoid recalculating the same thing many times.

```
      SUBROUTINE  SSU(I)                                                SSU       2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM     2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM     3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM     4
     +,NSM=4,NWPM=3729,NSD=NSM*NWPM+132,ML2=100)                        PARAM     5
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO INIT      2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT     3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)            INIT      4
      COMMON/VOID/INTX(ML2),JV(ML2),IV(ML2),NNV                         VD        2
      COMMON/EOSN/IEOS(ML),ME(ML)                                       EN        2
      COMMON/XCOM/R1,R2,DR1,DR2,WO,NCI,DR,ZI                            XC        2
      COMMON/NSPLT/NOSPLT(ML2)                                          NSP       2
      NAMELIST/SU/DTO,NOSPLT,IV,IEOS,MAT,ME,R1,R2,UO,NCI                NMLST     2
     +,DR1,DR2,UT,DTCF,IJK                                              NMLST     3
      NAMELIST/ESC/C1,S1,C2,S2,SWV,VMN,GAMMA,ALP,A,BR,BA,VBO,VBSW,      NMLST     4
     +FS,GS,HS,ST,SJ,CV,GC,SP,USP,CF,PS,BUA,BUB,BUMAX,BUDV,TMLT,TMC,    NMLST     5
     +XMU,YO,XL,XV,VO,PO,TO,ROW,PLAP,IBRN,NV,WO,ZI                      NMLST     6
     +,SR,ES,A1,A2,A3,EM,IRV,BUR,BUD,XISP,QO,IE                         NMLST     7
      NAMELIST/BURN/Z,E,VCJ,PCJ,DWDT,PM,ND                              NMLST     8
      NAMELIST/INP/NM,UI,UF,RO,IALPH,NDF,NI,NP,NG,NADD,NMAX,            NMLST     9
     +TEND,TP,TG,NDELT,UII,UFI,LABEL,NM1,IDMP,IV,NDUMP,TD,TFN           NMLST    10
      READ(5,SU)   Read SU namelist (data goes into region 1)           SSU      10
      J=I+1                                                             SSU      11
      DTO(J)=DTO(1)                                                     SSU      12
      NOSPLT(J)=NOSPLT(1)                                               SSU      13
      IV(J)=IV(1)                                                       SSU      14
      IEOS(J)=IEOS(1)                                                   SSU      15
      UO(J)=UO(1)                                                       SSU      16
      UT(J)=UT(1)                                                       SSU      17
      DTCF(J)=DTCF(1)                                                   SSU      18
      MAT(J)=MAT(1)                                                     SSU      19
      ME(J)=ME(1)                                                       SSU      20
      RETURN                                                            SSU      21
      END                                                               SSU      22
```

Copy all of the data into region I + 1

SSU(I)

Reads the SU namelist and copies material data to region I+1. (In order to keep the namelist variable names the same as those used in the code and at the same time avoid requiring region number subscripts in the input, region number one (i.e., no subscript) is used in the namelist. The data is then copied to region number I+1 where I is the actual region number. After all data is read in, every variable associated with regions has all of its data shifted down by one to the proper region. See subroutine RSTORE.)

Local Variables

J = I+1 is the region in which data is temporarily put (see above).

```
      SUBROUTINE ESSU(I)                                                ESSU      2
      COMMON/XCOM/R1,R2,DR1,DR2,WO,NCI,DR,ZI                            XC        2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM     2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM     3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM     4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                        PARAM     5
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO INIT      2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT     3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)            INIT      4
      COMMON/POLYC/CF(NCF,ML),PS(ML)                                    PLC       2
      COMMON/SPC/SP(ML),USP(ML)                                         SPLC      2
     +,XISP(ML)                                                         SPLC      3
      COMMON/USUPC/C1(ML),S1(ML),C2(ML),S2(ML),SWV(ML),VMN(ML),         US        2
     +GAMMA(ML),ALP(ML)                                                 US        3
      COMMON/BRNS/A(ML),BR(ML),BA(ML),VBO(ML),VBSW(ML)                  BRN       2
      COMMON/FGHIJC/FS(ML),GS(ML),HS(ML),SI(ML),SJ(ML),CV(ML)           FG        2
      COMMON/GASC/GC(NGC,ML)                                            GC        2
      COMMON/BUX/BUA,BUR,BUMAX,BUDV(ML)                                 BUP       2
     +,BUR,BUD                                                          BUP       3
      COMMON/EOSCOM/SR(ML),ES(ML),A1(ML),A2(ML),A3(ML),EM(ML),IRV(ML)   EOSCOM     2
      NAMELIST/SU/DTO,NOSPLT,IV,IEOS,MAT,ME,R1,R2,UO,NCI                NMLST     2
     +,DR1,DR2,UT,DTCF,IJK                                              NMLST     3
      NAMELIST/ESC/C1,S1,C2,S2,SWV,VMN,GAMMA,ALP,A,BR,BA,VBO,VBSW,      NMLST     4
     +FS,GS,HS,ST,SJ,CV,GC,SP,USP,CF,PS,BUA,BUB,BUMAX,BUDV,TMLT,TMC,    NMLST     5
     +XMU,YO,XL,XV,VO,PO,TO,ROW,PLAP,IBRN,NV,WO,ZI                      NMLST     6
     +,SR,ES,A1,A2,A3,EM,IRV,BUR,BUD,XISP,QO,IE                         NMLST     7
      NAMELIST/BURN/Z,E,VCJ,PCJ,DWDT,PM,ND                              NMLST     8
      NAMELIST/INP/NM,UI,UF,RO,IALPH,NDF,NI,NP,NG,NADD,NMAX,            NMLST     9
     +TEND,TP,TG,NDELT,UII,UFI,LABEL,NM1,IDMP,IV,NDUMP,TD,IFN           NMLST    10
      READ(5,ESC)   Read ESC namelist (data goes into region 1)         ESSU     17
      J=I+1                                                             ESSU     18
      C1(J)=C1(1)                                                       ESSU     19
      S1(J)=S1(1)                                                       ESSU     20
      C2(J)=C2(1)                                                       ESSU     21
      S2(J)=S2(1)                                                       ESSU     22
      SWV(J)=SWV(1)                                                     ESSU     23
      VMN(J)=VMN(1)                                                     ESSU     24
      GAMMA(J)=GAMMA(1)                                                 ESSU     25
      ALP(J)=ALP(1)                                                     ESSU     26
      A(J)=A(1)                                                         ESSU     27
      BR(J)=BR(1)                                                       ESSU     28
      BA(J)=BA(1)                                                       ESSU     29
      VBO(J)=VBO(1)                                                     ESSU     30
      VBSW(J)=VBSW(1)                                                   ESSU     31
      FS(J)=FS(1)           Copy ESC data into region I + 1             ESSU     32
      GS(J)=GS(1)                                                       ESSU     33
      HS(J)=HS(1)                                                       ESSU     34
      SI(J)=SI(1)                                                       ESSU     35
      SJ(J)=SJ(1)                                                       ESSU     36
      CV(J)=CV(1)                                                       ESSU     37
      SP(J)=SP(1)                                                       ESSU     38
      USP(J)=USP(1)                                                     ESSU     39
      PS(J)=PS(1)                                                       ESSU     40
      XMU(J)=XMU(1)                                                     ESSU     41
      YO(J)=YO(1)                                                       ESSU     42
      TMLT(J)=TMLT(1)                                                   ESSU     43
      TMC(J)=TMC(1)                                                     ESSU     44
      XL(J)=XL(1)                                                       ESSU     45
      XV(J)=XV(1)                                                       ESSU     46
      VO(J)=VO(1)                                                       ESSU     47
```

```
      PO(J)=PO(1)                                                ESSU      48
      QO(J)=QO(1)                                                ESSU      49
      TO(J)=TO(1)                                                ESSU      50
      ROW(J)=ROW(1)                                              ESSU      51
      PLAP(J)=PLAP(1)                                            ESSU      52
      IBRN(J)=IBRN(1)                                            ESSU      53
      NV(J)=NV(1)                                                ESSU      54
      BUDV(J)=BUDV(1)                                            ESSU      55
      DO 10 K=1,NGC                                              ESSU      56
   10 GC(K,J)=GC(K,1)                                            ESSU      57
      DO 20 K=1,NCF                                              ESSU      58
   20 CF(K,J)=CF(K,1)                                            ESSU      59
      SR(J)=SR(1)                                                ESSU      61
      ES(J)=ES(1)                                                ESSU      62
      A1(J)=A1(1)                                                ESSU      63
      A2(J)=A2(1)                                                ESSU      64
      A3(J)=A3(1)                                                ESSU      65
      EM(J)=EM(1)                                                ESSU      66
      IRV(J)=IRV(1)                                              ESSU      67
      RETURN                                                     ESSU      69
      END                                                        ESSU      70
```

ESSU(I)

Reads the ESC namelist (equation-of-state constants) and copies material data to region I+1.

Local Variables

J = I+1 is the region in which data is temporarily put.

K = do loop index.

NGC = the first dimension in the GC array = the number of gas constants allowed. (NGC is set in the parameter statement.)

NCF = the first dimension of the CF array = the number of parameters allowed in the 8-parameter fit. (NCF is set in the parameter statement.)

```
      SUBROUTINE BRSU(I)                                                BRSU      2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM     2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM     3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM     4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                        PARAM     5
      COMMON/BRND/Z(ML),E(ML),VCJ(ML),DWDT(NDW,ML),PCJ(ML),PM(ML),ND(ML) BRD     2
     +,MSFF                                                             BRD       3
      NAMELIST/SU/DTO,NOSPLT,IV,IEOS,MAT,ME,R1,R2,UO,NCI                NMLST     2
     +,DR1,DR2,UT,DTCF,IJK                                              NMLST     3
      NAMELIST/ESC/C1,S1,C2,S2,SWV,VMN,GAMMA,ALP,A,BR,BA,VBO,VBSW,      NMLST     4
     +FS,GS,HS,SI,SJ,CV,GC,SP,USP,CF,PS,BUA,BUB,BUMAX,BUDV,TMLT,TMC,    NMLST     5
     +XMU,YO,XL,XV,VO,PO,TO,ROW,PLAP,IBRN,NV,WO,ZI                      NMLST     6
     +,SR,ES,A1,A2,A3,EM,IRV,BUR,BUD,XISP,QO,IE                         NMLST     7
      NAMELIST/BURN/Z,E,VCJ,PCJ,DWDT,PM,ND                              NMLST     8
      NAMELIST/INP/NM,UI,UF,RO,IALPH,NDF,NI,NP,NG,NADD,NMAX,            NMLST     9
     +TEND,TP,TG,NDELT,UII,UFI,LABEL,NM1,IDMP,IV,NDUMP,TD,IFN           NMLST    10
      READ(5,BURN)  Read BURN namelist (data goes into region 1)        BRSU      6
      J=I+1                                                             BRSU      7
      Z(J)=Z(1)                                                         BRSU      8
      E(J)=E(1)                                                         BRSU      9
      VCJ(J)=VCJ(1)   Copy all BURN data into region I + 1              BRSU     10
      PCJ(J)=PCJ(1)                                                     BRSU     11
      PM(J)=PM(1)                                                       BRSU     12
      ND(J)=ND(1)                                                       BRSU     13
      DO 10 K=1,NDW                                                     BRSU     14
   10 DWDT(K,J)=DWDT(K,1)                                               BRSU     15
      RETURN                                                            BRSU     16
      END.                                                              BRSU     17
```

BRSU(I)

Reads the BURN namelist (various burn constants) and copies material data to region I+1.

Local Variables

J = I+1 is the region in which data is temporarily put.

K = do loop index.

NDW = the first dimension of the DWDT array = the number of Forest Fire constants allowed for each material. (NDW is set by the parameter statement.)

```
      SUBROUTINE CLR                                                    CLR        2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM      2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM      3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM      4
     +,NSM=4,NWPM=3729,NSD=NSM*NWPM+132,ML2=100)                        PARAM      5
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO INIT       2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT     3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)            INIT       4
      COMMON/USUPC/C1(ML),S1(ML),C2(ML),S2(ML),SWV(ML),VMN(ML),         US         2
     +GAMMA(ML),ALP(ML)                                                 US         3
      COMMON/BRND/Z(ML),E(ML),VCJ(ML),DWDT(NDW,ML),PCJ(ML),PM(ML),ND(ML) BRD      2
     +,MSFF                                                             BRD        3
      COMMON/GASC/GC(NGC,ML)                                            GC         2
      COMMON/FGHIJC/FS(ML),GS(ML),HS(ML),SI(ML),SJ(ML),CV(ML)           FG         2
      COMMON/VOID/INTX(ML2),JV(ML2),IV(ML2),NNV                         VD         2
      COMMON/BRNS/A(ML),BR(ML),BA(ML),VBO(ML),VBSW(ML)                  BRN        2
      COMMON/EOSN/IEOS(ML),ME(ML)                                       EN         2
      COMMON/NSPLT/NOSPLT(ML2)                                          NSP        2
      COMMON/SPC/SP(ML),USP(ML)                                         SPLC       2
     +,XISP(ML)                                                         SPLC       3
      COMMON/POLYC/CF(NCF,ML),PS(ML)                                    PLC        2
      COMMON/BUX/BUA,BUB,BUMAX,BUDV(ML)                                 BUP        2
     +,BUR,BUD                                                          BUP        3
      COMMON/XCOM/R1,R2,DR1,DR2,WO,NCI,DR,ZI                            XC         2
      COMMON/EOSCOM/SR(ML),ES(ML),A1(ML),A2(ML),A3(ML),EM(ML),TRV(ML)   EOSCOM      2
      DTO(1)=1.                                                         CLR       20
      NOSPLT(1)=0                                                       CLR       21
      IV(1)=-1          Reinitialize all variables in namelists         CLR       22
      UO(1)=0.          SU, ESC, and BURN (for region 1) to the default values  CLR  23
      UT(1)=1.E-10                                                      CLR       24
      DTCF(1)=0.5                                                       CLR       25
      IEOS(1)=1                                                         CLR       26
      MAT(1)=0                                                          CLR       27
      ME(1)=0                                                           CLR       28
      R2=0.                                                             CLR       29
      NCI=0                                                             CLR       30
      C1(1)=0.                                                          CLR       31
      S1(1)=0.                                                          CLR       32
      C2(1)=0.                                                          CLR       33
      S2(1)=0.                                                          CLR       34
      SWV(1)=0.                                                         CLR       35
      VMN(1)=0.                                                         CLR       36
      GAMMA(1)=0.                                                       CLR       37
      ALP(1)=0.                                                         CLR       38
      A(1)=0.                                                           CLR       39
      BR(1)=0.                                                          CLR       40
      BA(1)=0.                                                          CLR       41
      VBO(1)=0.                                                         CLR       42
      VBSW(1)=0.                                                        CLR       43
      FS(1)=0.                                                          CLR       44
      GS(1)=0.                                                          CLR       45
      HS(1)=0.                                                          CLR       46
      SI(1)=0.                                                          CLR       47
      SJ(1)=0.                                                          CLR       48
      CV(1)=0.                                                          CLR       49
      SP(1)=0.                                                          CLR       50
      USP(1)=0.                                                         CLR       51
      PS(1)=0.                                                          CLR       52
      BUDV(1)=0.                                                        CLR       53
      BUA=0.                                                            CLR       54
```

```
      BUB=0.                                                    CLR        55
      WO=1.                                                     CLR        56
      ZI=0.                                                     CLR        57
      XMU(1)=0.                                                 CLR        58
      YO(1)=0.                                                  CLR        59
      TMLT(1)=0.                                                CLR        60
      TMC(1)=0.                                                 CLR        61
      XL(1)=0.                                                  CLR        62
      XV(1)=2.                                                  CLR        63
      VO(1)=0.                                                  CLR        64
      PO(1)=1.E-10                                              CLR        65
      QO(1)=1.E-10                                              CLR        66
      TO(1)=0.                                                  CLR        67
      ROW(1)=0.                                                 CLR        68
      PLAP(1)=0.                                                CLR        69
      IBRN(1)=0                                                 CLR        70
      NV(1)=1                                                   CLR        71
      BUMAX=0.                                                  CLR        72
      DO 100 K=1,NGC                                            CLR        73
  100 GC(K,1)=0.                                                CLR        74
      DO 200 K=1,NCF                                            CLR        75
  200 CF(K,1)=0.                                                CLR        76
      Z(1)=0.                                                   CLR        77
      E(1)=0.                                                   CLR        78
      VCJ(1)=0.                                                 CLR        79
      PCJ(1)=0.                                                 CLR        80
      PM(1)=0.                                                  CLR        81
      ND(1)=0                                                   CLR        82
      DO 300 K=1,NDW                                            CLR        83
  300 DWDT(K,1)=0.                                              CLR        84
      SR(1)=1.                                                  CLR        86
      ES(1)=0.                                                  CLR        87
      A1(1)=0.                                                  CLR        88
      A2(1)=0.                                                  CLR        89
      A3(1)=0.                                                  CLR        90
      EM(1)=0.                                                  CLR        91
      IRV(1)=0                                                  CLR        92
      RETURN                                                    CLR        94
      END                                                       CLR        95
```

CLR

Resets region 1 data to the default values.

Local Variables

K = do loop index.

NGC = the first dimension in the GC array = the number of gas constants allowed. (NGC is set in the parameter statement.)

NCF = the first dimension in the CF array = the number of parameters allowed in the 8-parameter fit. (NCF is set in the parameter statement.)

NDW = the first dimension in the DWDT array = the number of Forest Fire constants allowed for each material. (NDW is set in the parameter statement.)

Notes

Default values must be included here as well as in the data statements in SETUP. (For data read in from disk, values are stored directly into region I+1. However, if more data is to be read from namelists, then the default values have to be reset in region 1 before the disk read is made.)

```
      SUBROUTINE RSTORE                                                 RSTORE     2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM      2
     +NUMV=10,MOL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM      3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM      4
     +,NSM=4,NWPM=372R,NSD=NSM*NWPM+132,ML2=100)                        PARAM      5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                         MCELL      2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)   MCELL      3
     +,W(MCL)                                                           MCELL      4
      LEVEL 2,R                                                         MCELL      5
      COMMON/DVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM, MCELL      6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                    MCELL      7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                  MCELL      8
      LEVEL 2,TIME                                                      MCELL      9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO  INIT       2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT       3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)            INIT       4
      COMMON/USUPC/C1(ML),S1(ML),C2(ML),S2(ML),SWV(ML),VMN(ML),         US         2
     +GAMMA(ML),ALP(ML)                                                 US         3
      COMMON/BRND/Z(ML),E(ML),VCJ(ML),DWDT(NDW,ML),PCJ(ML),PM(ML),ND(ML) BRD       2
     +,MSFF                                                             BRD        3
      COMMON/GASC/GC(NGC,ML)                                            GC         2
      COMMON/FGHIJC/FS(ML),GS(ML),HS(ML),SI(ML),SJ(ML),CV(ML)           FG         2
      COMMON/VOID/INTX(ML2),JV(ML2),IV(ML2),NNV                         VD         2
      COMMON/BRNS/A(ML),BR(ML),BA(ML),VBO(ML),VBSW(ML)                  BRN        2
      COMMON/EOSN/IEOS(ML),ME(ML)                                       EN         2
      COMMON/NSPLT/NOSPLT(ML2)                                          NSP        2
      COMMON/SPC/SP(ML),USP(ML)                                         SPLC       2
     +,XISP(ML)                                                         SPLC       3
      COMMON/POLYC/CF(NCF,ML),PS(ML)                                    PLC        2
      COMMON/BUY/BUA,BUB,BUMAX,BUDV(ML)                                 BUP        2
     +,BUR,BUD                                                          BUP        3
      COMMON/TABG/ESC(NTAB),NLOC(ML)                                    TABG       2
      COMMON/EOSCOM/SR(ML),ES(ML),A1(ML),A2(ML),A3(ML),EM(ML),IRV(ML)   EOSCOM     2
      DO 10 I=1,NM                                                      RSTORE    21
      J=I+1                                                             RSTORE    22
      DTO(I)=DTO(J)        Shift all variables in namelists            RSTORE    23
      XMU(I)=XMU(J)         SU, ESC, and BURN down one region          RSTORE    24
      YO(I)=YO(J)           to their proper place                      RSTORE    25
      TMLT(I)=TMLT(J)                                                   RSTORE    26
      TMC(I)=TMC(J)                                                     RSTORE    27
      XL(I)=XL(J)                                                       RSTORE    28
      XV(I)=XV(J)                                                       RSTORE    29
      VO(I)=VO(J)                                                       RSTORE    30
      PO(I)=PO(J)                                                       RSTORE    31
      QO(I)=QO(J)                                                       RSTORE    32
      TO(I)=TO(J)                                                       RSTORE    33
      ROW(I)=ROW(J)                                                     RSTORE    34
      PLAP(I)=PLAP(J)                                                   RSTORE    35
      IBRN(I)=IBRN(J)                                                   RSTORE    36
      NV(I)=NV(J)                                                       RSTORE    37
      NOSPLT(I)=NOSPLT(J)                                               RSTORE    38
      IV(I)=IV(J)                                                       RSTORE    39
      UO(I)=UO(J)                                                       RSTORE    40
      UT(I)=UT(J)                                                       RSTORE    41
      DTCF(I)=DTCF(J)                                                   RSTORE    42
      IEOS(I)=IEOS(J)                                                   RSTORE    43
      MAT(I)=MAT(J)                                                     RSTORE    44
      ME(I)=ME(J)                                                       RSTORE    45
      C1(I)=C1(J)                                                       RSTORE    46
      S1(I)=S1(J)                                                       RSTORE    47
```

```
      C2(I)=C2(J)                                                       RSTORE     48
      S2(I)=S2(J)                                                       RSTORE     49
      SWV(I)=SWV(J)                                                     RSTORE     50
      VMN(I)=VMN(J)                                                     RSTORE     51
      GAMMA(I)=GAMMA(J)                                                 RSTORE     52
      ALP(I)=ALP(J)                                                     RSTORE     53
      A(I)=A(J)                                                         RSTORE     54
      BR(I)=BR(J)                                                       RSTORE     55
      BA(I)=BA(J)                                                       RSTORE     56
      VBO(I)=VBO(J)                                                     RSTORE     57
      VBSW(I)=VBSW(J)                                                   RSTORE     58
      FS(I)=FS(J)                                                       RSTORE     59
      GS(I)=GS(J)                                                       RSTORE     60
      HS(I)=HS(J)                                                       RSTORE     61
      SI(I)=SI(J)                                                       RSTORE     62
      SJ(I)=SJ(J)                                                       RSTORE     63
      CV(I)=CV(J)                                                       RSTORE     64
      SP(I)=SP(J)                                                       RSTORE     65
      USP(I)=USP(J)                                                     RSTORE     66
      PS(I)=PS(J)                                                       RSTORE     67
      BUDV(I)=BUDV(J)                                                   RSTORE     68
      DO 100 M=1,NGC                                                    RSTORE     69
  100 GC(M,I)=GC(M,J)                                                   RSTORE     70
      DO 200 M=1,NDW                                                    RSTORE     71
  200 DWDT(M,I)=DWDT(M,J)                                               RSTORE     72
      DO 300 M=1,NCF                                                    RSTORE     73
  300 CF(M,I)=CF(M,J)                                                   RSTORE     74
      Z(I)=Z(J)                                                         RSTORE     75
      E(I)=E(J)                                                         RSTORE     76
      VCJ(I)=VCJ(J)                                                     RSTORE     77
      PCJ(I)=PCJ(J)                                                     RSTORE     78
      PM(I)=PM(J)                                                       RSTORE     79
      ND(I)=ND(J)                                                       RSTORE     80
      DRO(I)=DRO(J)                                                     RSTORE     81
      NLOC(I)=NLOC(J)                                                   RSTORE     82
      SR(I)=SR(J)                                                       RSTORE     84
      ES(I)=ES(J)                                                       RSTORE     85
      A1(I)=A1(J)                                                       RSTORE     86
      A2(I)=A2(J)                                                       RSTORE     87
      A3(I)=A3(J)                                                       RSTORE     88
      EM(I)=EM(J)                                                       RSTORE     89
      IRV(I)=IRV(J)                                                     RSTORE     90
   10 CONTINUE                                                          RSTORE     92
      RETURN                                                            RSTORE     93
      END                                                               RSTORE     94
```

RSTORE

Shifts region I+1 data back to I (where it should be) for each region I.

Local Variables

K = do loop index.

NGC = the first dimension in the GC array - the number of gas constants allowed. (NGC is set in the parameter statement.)

NCF = the first dimension in the CF array = the number of parameters allowed in the 8-parameter fit. (NCF is set in the parameter statement.)

NDW = the first dimension in the DWDT array = the number of Forest Fire constants allowed for each material. (NDW is set in the parameter statement.)

```
      SUBROUTINE EOSDSK(I)                                              EOSDSK     2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*4L,         PARAM      2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM      3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM      4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                        PARAM      5
      COMMON/XEOS/IX                                                    XEOS       2
      COMMON/EOSN/IEOS(ML),ME(ML)                                       EN         2
      DATA IST/1/                                                       EOSDSK     6
      IF(IST.EQ.2)GO TO 2                                               EOSDSK     7
      IST=2                          1st time through                   EOSDSK     8
      CALL QASSIGN(22,5HSES2L,0,0)    QASSIGN all EOS files             EOSDSK    10
      CALL QASSIGN(23,4HHMLB,0,0)                                       EOSDSK    12
    2 CONTINUE                                                          EOSDSK    13
      IX=I+1                                                            EOSDSK    14
      ITYPE=IEOS(IX)                                                    EOSDSK    15
      GO TO (11,12,13,14),ITYPE                                         EOSDSK    16
   11 CALL RHOM                      Call the appropriate subroutine to read  EOSDSK    17
      RETURN                          and store data for that type of EOS   EOSDSK    18
   12 CALL RBLDUP                                                       EOSDSK    19
      RETURN                                                            EOSDSK    20
   13 CALL RPOLY                                                        EOSDSK    21
      RETURN                                                            EOSDSK    22
   14 CALL RSFSAME                                                      EOSDSK    23
      RETURN                                                            EOSDSK    24
      END                                                               EOSDSK    25
```

EOSDSK

Switching routine that assigns units for EOS files and calls routines to read them. (Data from EOS files can then be overridden by namelist reads.)

Local Variables

IST = flag to determine whether this is the first call to EOSDSK.

IX = I+1 = data is stored in region I+1 during setup.

ITYPE = IEOS for that region.

Notes

IX is used in all of the called subroutines.

```
      SUBROUTINE RHOM                                                   PHOM      2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM      2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM      3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM      4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                        PARAM      5
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO INIT       2
     +(ML),TO(ML),PDW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT      3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)            INIT       4
      COMMON/USUPC/C1(ML),S1(ML),C2(ML),S2(ML),SWV(ML),VMN(ML),         US         2
     +GAMMA(ML),ALP(ML)                                                 US         3
      COMMON/BRND/Z(ML),E(ML),VCJ(ML),DWDT(NDW,ML),PCJ(ML),PM(ML),ND(ML) BRD       2
     +,MSFF                                                             BRD        3
      COMMON/GASC/GC(NGC,ML)                                            GC         2
      COMMON/SPC/SP(ML),USP(ML)                                         SPLC       2
     +,XISP(ML)                                                         SPLC       3
      COMMON/FGHTJC/FS(ML),GS(ML),HS(ML),SI(ML),SJ(ML),CV(ML)           FG         2
      COMMON/BRNS/A(ML),BR(ML),BA(ML),VBO(ML),VBSW(ML)                  BRN        2
      COMMON/EOSN/IEOS(ML),ME(ML)                                       EN         2
      COMMON/BUX/BUA,BUB,BUMAX,BUDV(ML)                                 BUP        2
     +,BUR,BUD                                                          BUP        3
      COMMON/XEOS/IX                                                    XEOS       2
      DIMENSION DAT(84),IDAT(84),NAM(3)                                 RHOM      14
      EQUIVALENCE(DAT,IDAT)                                             RHOM      15
      DATA LUN/23/    Unit # for HMLB                                   RHOM      16
      I=IX                                                              RHOM      17
      NNA=3*MAT(I)-1   Location in index of 1st word address for material # MAT(I) RHOM  18
      CALL RDISK(LUN,NAM,3,NNA)  ]- Read the FWA plus two words of comment RHOM    19
      IF(UNIT(LUN))1,1,1         ]                                      RHOM      20
    1 CONTINUE                                                          RHOM      21
      CALL RDISK(LUN,DAT,84,NAM(1))] Read the 84 words of HOM data      RHOM      22
      IF(UNIT(LUN))2,2,2           ]                                    RHOM      23
    2 CONTINUE                                                          RHOM      24
      IBRN(I)=IDAT(4)                                                   RHOM      25
      IF(IBRN(I).LE.1)IBRN(I)=IBRN(I)+1                  ] Convert the SIN type RHOM  26
      IF(DAT(64).EQ.0..AND.IBRN(I).EQ.1)IBRN(I)=0        ]  burn index  RHOM      27
      IF(ME(I).EQ.0)GO TO 10  ]                                         RHOM      28
      IBRN(1)=IBRN(I)         ] If more data is to be read from namelist, then RHOM 29
      I=1                       the region 1 values must be set to override RHOM  30
   10 CONTINUE                  the default values                      RHOM      31
      NV(I)=IDAT(5)+1                                                   RHOM      32
      IF(NV(I).EQ.3)NV(I)=0                                             RHOM      33
      XV(I)=DAT(6)                                                      RHOM      34
      TO(I)=DAT(9)                                                      RHOM      35
      C1(I)=DAT(12)                                                     RHOM      36
      S1(I)=DAT(13)                                                     RHOM      37
      SWV(I)=DAT(14)                                                    RHOM      38
      C2(I)=DAT(15)          Load the data into the proper constants    RHOM      39
      S2(I)=DAT(16)                                                     RHOM      40
      FS(I)=DAT(17)                                                     RHOM      41
      GS(I)=DAT(18)                                                     RHOM      42
      HS(I)=DAT(19)                                                     RHOM      43
      SI(I)=DAT(20)                                                     RHOM      44
      SJ(I)=DAT(21)                                                     RHOM      45
      GAMMA(I)=DAT(22)                                                  RHOM      46
      CV(I)=DAT(23)                                                     RHOM      47
      ALP(I)=DAT(25)                                                    RHOM      48
      SP(I)=DAT(26)                                                     RHOM      49
      USP(I)=DAT(27)                                                    RHOM      50
      YO(I)=DAT(30)                                                     RHOM      51
      XMU(I)=DAT(31)                                                    RHOM      52
```

```
      PLAP(I)=DAT(32)                                                    RHOM      53
      VMN(I)=DAT(34)                                                     RHOM      54
      Z(I)=DAT(36)                                                       RHOM      55
      E(I)=DAT(37)                                                       RHOM      56
      TMLT(I)=E(I)                                                       RHOM      57
      TMC(I)=Z(I)                                                        RHOM      58
      VCJ(I)=DAT(38)                                                     RHOM      59
      ND(I)=IDAT(41)                                                     RHOM      60
      PCJ(I)=DAT(42)                                                     RHOM      61
      PM(I)=DAT(43)                                                      RHOM      62
      DO 110 K=1,20                                                      RHOM      63
110   DWDT(K,I)=DAT(K+43)                                                RHOM      64
      DO 111 K=1,17                                                      RHOM      65
111   GC(K,I)=DAT(K+63)                                                  RHOM      66
      A(I)=DAT(64)                                                       RHOM      67
      BR(I)=DAT(65)                                                      RHOM      68
      BA(I)=DAT(66)                                                      RHOM      69
      VBO(I)=DAT(67)                                                     RHOM      70
      VBSW(I)=DAT(68)                                                    RHOM      71
      ROW(I)=DAT(7)                                                      RHOM      72
      GC(18,I)=10.  ]                                                    RHOM      73
      GC(19,I)=-20. ] Default limits on the region of validity of two fits in MIX  RHOM  74
      IF(IBRN(I).EQ.4)CALL GASLM(I)  Calculate the actual limits of validity  RHOM  75
      RETURN                                                             RHOM      76
      END                                                                RHOM      77
```

RHOM

Reads EOS file HMLB to get HOM EOS data.

Local Variables

I = IX = temporary region # in which data is stored.

NNA = location in HMLB of the 1st word address for the location of data for the material # MAT(I).

NAM = three words in the index for material # MAT(I). Word #1 is the 1st word address described above. Words 2 and 3 are Hollerith data giving a label for that material.

DAT = the actual data (84 words) for that HOM material. The order corresponds to that in the SIN input deck for the same material.

IDAT = equivalenced to DAT, so that integer data can be retrieved without conversion.

JJ = an index such that data is stored in region 1 only if more namelist data is to be read (ME=1).

Notes

IBRN and NV require conversion from their corresponding SIN values.

Data is stored directly in region I+1 if no changes are to be made (ME = 0).

Data is stored in region 1 if changes are to be made by namelist (ME $\neq$ 0).

After changes are made, all of the region 1 data is copied to region I+1.

```
      SUBROUTINE RBLDUP                                                 RBLDUP     2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM      2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM      3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM      4
     +,NSM=4,NWPM=3729,NSD=NSM*NWPM+132,ML2=100)                        PARAM      5
      COMMON/BUX/BUA,BUB,BUMAX,BUDV(ML)                                 BUP        2
     +,BUR,BUD                                                          BUP        3
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                         MCELL      2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)   MCELL      3
     +,W(MCL)                                                           MCELL      4
      LEVEL 2,R                                                         MCELL      5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UTI,UFT,NADD,NM, MCELL      6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                    MCELL      7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                  MCELL      8
      LEVEL 2,TIME                                                      MCELL      9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO  INIT       2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT       3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)            INIT       4
      COMMON/XEOS/IX                                                    XEOS       2
      COMMON/EOSN/IEOS(ML),ME(ML)                                       EN         2
      DIMENSION DAT(84),IDAT(84),NAM(3)                                 RBLDUP     9
      EQUIVALENCE(DAT,IDAT)                                             RBLDUP    10
      DATA LUN/23/                                                      RBLDUP    11
      I=IX                                                              RBLDUP    12
      NNA=3*MAT(I)-1                                                    RBLDUP    13
      CALL RDISK(LUN,NAM,3,NNA)                                         RBLDUP    14
      IF(UNIT(LUN))1,1,1                                                RBLDUP    15
    1 CONTINUE                                                          RBLDUP    16
      CALL RDISK(LUN,DAT,84,NAM(1))                                     RBLDUP    17
      IF(UNIT(LUN))2,2,2                                                RBLDUP    18
    2 CONTINUE                                                          RBLDUP    19
      BUA=DAT(81)                                                       RBLDUP    20
      BUB=DAT(82)                                                       RBLDUP    21
      BUMAX=DAT(83)                                                     RBLDUP    22
      IF(ME(I).NE.0)I=1                                                 RBLDUP    23
      BUDV(I)=DAT(84)                                                   RBLDUP    24
      IBRN(I)=2                                                         RBLDUP    25
      ROW(I)=DAT(7)                                                     RBLDUP    26
      NV(I)=IDAT(5)+1                                                   RBLDUP    27
      IF(NV(I).EQ.3)NV(I)=0                                             RBLDUP    28
      XV(I)=DAT(6)                                                      RBLDUP    29
      RETURN                                                            RBLDUP    30
      END                                                               RBLDUP    31
```

See RHOM

Load the data into the proper constants

RBLDUP

Reads EOS file HMLB to get data for the buildup EOS and burn model.

Local Variables

I = IX = temporary region # in which data is stored.

NNA = location in HMLB of the 1st word address for the location of data for the material # MAT(I).

NAM = the 3 words in the index for material # MAT(I). Work #1 is the 1st word address described above. Words 2 and 3 are Hollerith data giving a label for that material.

DAT = the actual data (84 words) for that HOM material. The order corresponds to that in the SIN input deck for the same material.

IDAT = equivalenced to DAT, so that integer data can be retrieved without conversion.

JJ = an index such that data is stored in region 1 only if more namelist data is to be read (ME=1).

Notes

NV requires conversion from the corresponding SIN value. See notes for RHOM.

```
      SUBROUTINE RPOLY                                                  RPOLY      2
      PRINT 900                                                         RPOLY      3
      WRITE(5,900)                                                      RPOLY      4
      WRITE(6,900)                                                      RPOLY      5
      WRITE(9,900)                    Output message and STOP           RPOLY      6
  900 FORMAT(1X,20H**********************/                            RPOLY      7
     +1X,20H*  NO LIBRARY FOR  */                                       RPOLY      8
     +1X,20H* IFOS=3 MATERIALS */                                       RPOLY      9
     +1X,20H**********************)                                   RPOLY     10
      STOP                                                              RPOLY     11
      END                                                               RPOLY     12
```

RPOLY

Dummy routine because a library is not provided for the eight-parameter fit constants.

```
      SUBROUTINE RSESAME                                                RSESAME    2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM      2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM      3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM      4
     +,NSM=4,NWPM=3729,NSD=NSM*NWPM+132,ML2=100)                        PARAM      5
      LEVEL 2,DC                                                        RSESAME    5
      COMMON/SESDAT/DC(NSD)                                             RSESAME    6
      COMMON/S2DIR/LCMX,NREG,LCFW(ML,1)                                 S2DIR      2
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO INIT       2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT     3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QQ(ML),TMLT(ML),TMC(ML)            INIT       4
      COMMON/XEOS/IX                                                    XEOS       2
      DIMENSION ZB(3)                                                   RSESAME   10
      DATA LCNT/1/                                                      RSESAME   11
      DATA LU1,LU2/21,22/   Unit # for SES2L                            RSESAME   12
      IR=IX-1   Region # is what it will be after RSTORE is called      RSESAME   13
      IF(LCNT.GT.1) GO TO 10                                            RSESAME   14
      NREG=ML                                                           RSESAME   15
      LCMX=NSD                  Initialize                              RSESAME   16
      DO 5 I=1,NREG                                                     RSESAME   17
      LCFW(I,1)=0                                                       RSESAME   18
 5    CONTINUE                                                          RSESAME   19
 10   CALL GETINV(IR,MAT(IX),1,DC,LCNT,LU2,IFL,ZB)  Store data          RSESAME   20
      IF(IFL.LT.0) GO TO 90                                             RSESAME   21
      IF(IFL.GT.0) GO TO 100                                            RSESAME   22
      PRINT 20,MAT(IX)                                                  RSESAME   23
 20   FORMAT(* SESAME MATERIAL * ,I5, * NOT FOUND *)                    RSESAME   24
      RETURN                                                            RSESAME   25
 90   PRINT 95,MAT(IX)                                                  RSESAME   26
 95   FORMAT(* NOT ENOUGH STORAGE SPACE TO LOAD SESAME MATERIAL *,      RSESAME   27
     $ I5)                                                              RSESAME   28
      RETURN                                                            RSESAME   29
C . . MATERIAL LOADED                                                   RSESAME   30
 100  ROW(IX)=DC(LCFW(IR,1)+1)  Get density from SESAME                 RSESAME   31
      ROW(1)=ROW(IX)                                                    RSESAME   32
      RETURN                                                            RSESAME   33
      END                                                               RSESAME   46
```

RSESAME

Reads data from disk for SESAME materials.

Local Variables

I = do loop index.

IFL = error flag, see GETINV.

IR = region #.

LCNT = position in array for storing tables, see GETINV.

LU2 = unit # for reading SESAME library.

ZB = output array from GETINV that is not used.

Notes

Calls GETINV of the SESAME package to initialize data. If SESAME is not defined (*DEFINE SESAME not in the update input file), a message is returned to the terminal and all print files that a compilation including SESAME is required to run a problem with a SESAME EOS. Execution of the program then terminates. Sample update commands to define SESAME are given below:

```
*ID SMDF
*B MAIN.1
*DEFINE SESAME
```

```
      SUBROUTINE JMNMX(NMAX)                                                    JMNMX      2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,                 PARAM      2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                          PARAM      3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                            PARAM      4
     +,NSM=4,NWPM=3729,NSD=NSM*NWPM+132,ML2=100)                                PARAM      5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                                 MCELL      2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)          MCELL      3
     +,W(MCL)                                                                   MCELL      4
      LEVEL 2,R                                                                 MCELL      5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM,         MCELL      6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TO(ML),TJK                            MCELL      7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                          MCELL      8
      LEVEL 2,TIME                                                              MCELL      9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),YV(ML),NV(ML),VO(ML),PO         INIT       2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML),       INIT       3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QQ(ML),TMLT(ML),TMC(ML)                    INIT       4
      COMMON/MNMX/KMAX(ML2),KMIN(ML2),NMC                                       MN         2
      COMMON/ES/IE(ML2),NME                                                     ESM        2
      DATA IST/1/,NMC/1/                                                        JMNMX      8
      IF(IST.NE.1) GO TO 2                                                      JMNMX      9
      IST=2                                                                     JMNMX     10
      IF(TIME.NE.0..AND.NM1.EQ.1)GO TO 2  Don't set KMIN,KMAX for a restart     JMNMX     11
      DO 1 I=NM1,NM                        unless there are changes             JMNMX     12
      KMAX(I)=JMAX(I)                                                           JMNMX     13
      KMIN(I)=JMIN(I)                                                           JMNMX     14
    1 CONTINUE                                                                  JMNMX     15
      NME=NM                                                                    JMNMX     16
    2 CONTINUE                                                                  JMNMX     17
      JM=0                                                                      JMNMX     18
      IF(NMAX.GT.KMAX(NM))NMAX=KMAX(NM)                                         JMNMX     19
      DO 10 I=NMC,NM                                                            JMNMX     20
      IF(JM.NE.0) GO TO 10                                                      JMNMX     21
      IF(NMAX.GT.KMAX(I)) GO TO 10                                              JMNMX     22
      JM=I                                 Reset JMAX's to correspond           JMNMX     23
   10 CONTINUE                              to NMAX active cells                JMNMX     24
      IF(JM.EQ.0) JM=NMC                                                        JMNMX     25
      IF(JM.NE.NMC) JMAX(NMC)=KMAX(NMC)                                         JMNMX     26
      NMC=JM                                                                    JMNMX     27
      JMAX(NMC)=NMAX                                                            JMNMX     28
      IF(NMAX.LT.JMIN(NMC)) JMAX(NMC)=JMIN(NMC)                                 JMNMX     29
      RETURN                                                                    JMNMX     30
      END                                                                       JMNMX     31
```

JMNMX(NMAX)

Sets indices to determine the minimum and maximum cell numbers for each material. Also sets indices for the last region with a cell turned on and the last cell turned on.

Local Variables

NMAX = cell # of the last cell turned on (subroutine argument).

IST = index that is 1 the 1st time through and 2 thereafter.

I = do loop index = region #.

JM = variable used to find the region which NMAX is in and reset NMC if necessary.

Notes

The first time through, KMIN and KMAX are set to JMIN and JMAX which were determined in SETUP. If the problem has been restarted (TIME $\neq$ 0 the 1st time through) and no changes have been made (NM1 = 1), then it is not necessary to change KMIN and KMAX. In the current usage, KMIN is always the same as JMIN. KMAX is the same as JMAX except for the last region that is turned on. In that case, JMAX is the last cell turned on in the region and KMAX is the last cell in the region.

Each time through, a test is made to determine which region NMAX is in. JMAX for that region is set to NMAX. Sometimes NMAX will be the cell number of an artificial cell used for voids. In that case, JMAX of the next region is set to JMIN. Also, the index NMC (which is the region number of the last active region) is reset accordingly. See SHFT for the effects of spalling and rezoning on the cell numbering.

```
      SUBROUTINE HEI(I)                                                 HEI        2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM      2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM      3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM      4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                        PARAM      5
      COMMON/ES/IE(ML2),NME                                             ESM        2
      COMMON/GASC/GC(NGC,ML)                                            GC         2
      COMMON/BUX/BUA,BUB,BUMAX,BUDV(ML)                                 BUP        2
     +,BUR,BUD                                                          BUP        3
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO INIT       2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT     3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)            INIT       4
      COMMON/EOSN/IEOS(ML),ME(ML)                                       EN         2
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                         MCELL      2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)   MCELL      3
     +,W(MCL)                                                           MCELL      4
      LEVEL 2,R                                                         MCELL      5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM, MCELL      6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                    MCELL      7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                  MCELL      8
      LEVEL 2,TIME                                                      MCELL      9
      DIMENSION G(1)                                                    HEI       10
      EQUIVALENCE (G,GC)                                                HEI       11
      IM=I-1                                                            HEI       12
      JMN=JMIN(IM)                                                      HEI       13
      JMX=JMAX(IM)                                                      HEI       14
      GO TO (1,2,99,99),IEOS(I)                                         HEI       15
    1 CONTINUE    HOM EOS                                             HEI       16
      K=IM*NGC                                                          HEI       17
      XMT=0.                                                            HEI       18
      DO 11 J=JMN,JMX                                                   HEI       19
   11 XMT=XMT+XM(J)    Total mass                                       HEI       20
      X=G(K+19)                                                         HEI       21
      EE(3*ML+IM)=(EXP(G(K+6)+X*(G(K+7)+X*(G(K+8)+X*(G(K+9)+X*G(K+10)   HEI       22
     +))))-G(K+17))*XMT   Reference energy for very large volumes       HEI       23
      RETURN                                                            HEI       24
    2 CONTINUE    BLDUP EOS                                           HEI       25
      EB=0.                                                             HEI       26
      DO 10 J=JMN,JMX                                                   HEI       27
   10 EB=EB+XM(J)/(T(J)*T(J)-1.)    Σ Mj/(γj² - 1)                     HEI       28
      EE(3*ML+IM)=EB*BUDV(I)/2    Σ MjD²/[2(γj² - 1)]                   HEI       29
      RETURN                                                            HEI       30
   99 EE(ML*3+IM)=0.    No shift calculated                            HEI       31
      RETURN                                                            HEI       32
      END                                                               HEI       33
```

HEI

Calculates the total internal energy of a region of solid HE relative to the energy of its products at infinite expansion at T = 0.

Local Variables

EB = the sum over cells in the region of $M_j/(\gamma^2 - 1)$.

IM = I - 1 = the actual region # (EOS data is still stored in the region # + 1 when HEI is called).

JMN, JMX = minimum and maximum cell # in the region.

K = index to locate the data for this region in G.

G = gas constants for a HOM gas.

X = ℓn P at which the reference energy is set to a constant (see GASLM).

XMT = total "mass" in a region.

Notes

The total internal energy at infinite expansion for HE products is calculated for each region that is an HE. This constant is used to shift the total energy and total internal energy calculations for those regions. The shifted energies are relative to the infinite expansion energy and, therefore, reflect how much energy has not been transferred from the HE to other regions in the system.

For the HOM EOS the reference energy becomes a constant calculated in GASLIM for very large volumes. This value is used for the infinite expansion energy.

For Buildup EOS, the infinite expansion energy becomes

$$K = -\frac{D^2}{2(\gamma^2 - 1)} \quad ,$$

because the γ-law energy term goes to zero at large volume. Since γ is not the same for all cells, the sum of the energy in each cell is calculated.

```
      SUBROUTINE GASLM(I)                                                GASLM     2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,          PARAM     2
     +NUMV=10,MQI=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                   PARAM     3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                     PARAM     4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                         PARAM     5
      COMMON/GASC/GC(NGC,ML)                                             GC        2
      EQUIVALENCE (GC,G)                                                 GASLM     5
      DIMENSION G(MLGC)                                                  GASLM     6
      K=(I-1)*NGC                                                        GASLM     7
      IF(G(K+15).EQ.0.)GO TO 15                                          GASLM     8
      TU=G(K+14)/(4*G(K+15))          General case for -1/β              GASLM     9
      G(K+18)=-TU+SQRT(TU*TU-G(K+13)/(6*G(K+15)))                        GASLM    10
      GO TO 14                                                           GASLM    11
   15 CONTINUE                                                           GASLM    12
      IF(G(K+14).EQ.0.)GO TO 14                                          GASLM    13
      G(K+18)=G(K+13)/(3*G(K+14))   Special case for U = 0               GASLM    14
   14 CONTINUE                                                           GASLM    15
      IF(G(K+10).EQ.0.)GO TO 10                                          GASLM    16
      P=0.75*G(K+9)/G(K+10)                                              GASLM    17
      Q=0.5*G(K+8)/G(K+10)                                               GASLM    18
      R=0.25*G(K+7)/G(K+10)                                              GASLM    19
      A=(3*Q-P*P)/3                   General case for &n I              GASLM    20
      B=(2*P*P*P-9*P*Q+27*R)/27                                          GASLM    21
      SBA=SQRT(B*B/4+A*A*A/27)                                           GASLM    22
      OT=1./3.                                                           GASLM    23
      BT=-B/2                                                            GASLM    24
      BTMS=BT-SBA                                                        GASLM    25
      BTPS=BT+SBA                                                        GASLM    26
      G(K+19)=SIGN(1.,BTPS)*ABS(BTPS)**OT+SIGN(1.,BTMS)*ABS(BTMS)**OT    GASLM    27
     +-P/3                                                               GASLM    28
      RETURN                                                             GASLM    29
   10 CONTINUE                                                           GASLM    30
      IF(G(K+9).EQ.0.)GO TO 9  Special case for O = 0                    GASLM    31
      G(K+19)=(-2*G(K+8)+SQRT(4*G(K+8)**2-12*G(K+9)*G(K+7)))/(6*G(K+9))  GASLM    32
      RETURN                                                             GASLM    33
    9 CONTINUE                                                           GASLM    34
      IF(G(K+8).EQ.0.)GO TO 8                                            GASLM    35
      G(K+19)=G(K+7)/(2*G(K+8))   Special case for O = N = 0             GASLM    36
    8 CONTINUE                                                           GASLM    37
      RETURN                                                             GASLM    38
      END                                                                GASLM    39
```

GASLM(I)

Finds limits for the region in which two of the analytic fits in GAS are reasonable.

Local Variables

G = equivalenced to GC but only one index.

K = Index to find the proper location in the G array for region I.

TU,P,Q,R,A,B = defined in notes below.

$SBA = \sqrt{\frac{B^2}{4} + \frac{A^3}{27}}$.

OT = 1/3.

BT = -B/2.

BTMS = BT - SBA.

Notes

Two of the analytic fits in GAS can cause problems in regions of high specific volume (typically $\approx 10\ V_0 - 100\ V_0$). In most problems the volumes will be small enough for the fits to be good during the time of interest. However, in cases where an HE decomposes a few percent and then expands, most of the expansion is done by the product gas. This situation can lead to very large volumes for the gas even though the specific volume of the mixture is still $\approx 2\ V_0$.

The fits that cause problems are

$$-\frac{1}{\beta} = R + 2S(\ln V) + 3T(\ln V)^2 + 4U(\ln V)^3 \qquad (1)$$

and

$$\ln I_i' = K + L(\ln P_i) + M(\ln P_i)^2 + N(\ln P_i)^3 + O(\ln P_i)^4 \quad . \qquad (2)$$

For a typical choice of constants, the fit to $-\frac{1}{\beta}$ has a relative minimum and a relative maximum. For large V, the cubic term dominates and $-\frac{1}{\beta}$ becomes very large. In the Grüneisen EOS,

$$P = \frac{1}{\beta V} (I - I_i) + P_i \quad , \tag{3}$$

a large $-\frac{1}{\beta}$ gives large vlaues of $|P|$ in a region where it should be small. We have artificially chosen V at the second extremum (denoted V_2) to be the largest value of V at which the fit in Eq. (1) will be used. For larger V, the value of $-\frac{1}{\beta}$ at V_2 is used.

The extrema can be found at the zeros of $\frac{d}{dV}(-\frac{1}{\beta})$, i.e., solve the equation

$$\frac{d}{dV} (R + 2S(\ell n\ V) + 3T(\ell n\ V)^2 + 4U(\ell n\ V)^3) = 0 \tag{4}$$

to find the values of $\ell n\ V$ at the extrema. Eq. (4) simplifies to

$$\frac{S}{6U} + \frac{T}{2U} \ell n\ V + (\ell n\ V)^2 = 0 \quad , \tag{5}$$

which has the solutions

$$\ell n\ V = \frac{-\frac{T}{2U} \pm \sqrt{\left(\frac{T}{2U}\right)^2 - 4\left(\frac{S}{6U}\right)}}{2} \quad . \tag{6}$$

We will use the greater of the two which is

$$\ell n\ V_2 = -\frac{T}{4U} + \sqrt{\left(\frac{T}{4U}\right)^2 - \frac{S}{6U}} \quad . \tag{7}$$

For a typical choice of constants, the fit to $\ell n\ I_i$ has one extremum, which is found by solving

$$\frac{d}{d(\ell n\ P)} [K + L(\ell n\ P) + M(\ell n\ P)^2 + N(\ell n\ P)^3 + O(\ell n\ P)^4] = 0 \tag{8}$$

or

$$L + 2M(\ell n\ P) + 3N(\ell n\ P)^2 + 4O(\ell n\ P)^3 = 0 \quad . \tag{9}$$

In the CRC Standard Math Tables we see that the general cubic equation, $y^3 + Py^2 + Qy + R = 0$, may be put in the form

$$x^3 + Ax + B = 0 \quad , \tag{10}$$

where

$$x = y + \frac{P}{3} \quad , \tag{11}$$

$$A = \frac{1}{3}\,(3Q - P^2) \quad , \tag{12}$$

and

$$B = \frac{1}{27}\,(2P^3 - 9PQ + 27R) \quad . \tag{13}$$

The real solution for the case where there is one real root is given by

$$x = \sqrt[3]{-\frac{B}{2} + \sqrt{\frac{B^2}{4} + \frac{A^3}{27}}} + \sqrt[3]{-\frac{B}{2} - \sqrt{\frac{B^2}{4} + \frac{A^3}{27}}} \quad . \tag{14}$$

```
      FUNCTION BLDSM(DR,I)                                                BLDSM     2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,           PARAM     2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                    PARAM     3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                      PARAM     4
     +,NSM=4,NWPM=3729,NSD=NSM*NWPM+132,ML2=100)                          PARAM     5
      COMMON/BUX/BUA,BUB,BUMAX,BUDV(ML)                                   BUP       2
     +,BUR,BUD                                                            BUP       3
      DATA IL/0/                                                          BLDSM     5
      IF(BUD.LE.0.)GO TO 2                                                BLDSM     6
      IF(I.EQ.IL)GO TO 1                                                  BLDSM     7
      IL=I                                                                BLDSM     8
      XX=BUB/(BUMAX-BUA)                                                  BLDSM     9
      B=XX-BUD                                                            BLDSM    10
      X=(3*BUB+SQRT(9*BUB*BUB-8*(BUMAX-BUA)*BUB*B))/                      BLDSM    11
     +(4*(BUMAX-BUA))                                                     BLDSM    12
      A=BUB/(2*(X-B)*X*X)                                                 BLDSM    13
    1 CONTINUE                                                            BLDSM    14
      IF(DR.LT.B.OR.DR.GT.X)GO TO 2                                       BLDSM    15
      BLDSM=BUMAX-A*(DR-B)**2  Evaluate smoothing function                BLDSM    16
      RETURN                                                              BLDSM    17
    2 CONTINUE                                                            BLDSM    18
      BLDSM=BUA+BUR/DR                                                    BLDSM    19
      IF(BLDSM.GT.BUMAX)BLDSM=BUMAX                                       BLDSM    20
      RETURN                                                              BLDSM    21
      END                                                                 BLDSM    22
```

Set up smoothing function

Usual functional form of γ

BLDSM

Calculates the γ for each cell using the buildup model. The transition from constant γ_{max} to the $\gamma = A + B/R$ form is smoothed out with a parabola which joins both curves, leaving the first derivative continuous.

Local Variables

A = a in notes.

B = b in notes.

IL = last region #.

X = X in notes.

XX = X_0 in notes.

Notes

The γ used in the buildup model is a function of the form

$$\gamma = \text{Min } (A + B/R, \gamma_{max}) \quad . \tag{1}$$

This function has a discontinuous first derivative at

$$X_0 = \frac{B}{\gamma_{max} - A} \quad . \tag{2}$$

For some cases this can cause a perturbation in the numerical solution that is eliminated by smoothing out the discontinuity. A convenient way to smooth out the discontinuity is to find a parabola with the following properties. (1) It intersects the line $\gamma = \gamma_{max}$ at $R = X_0 - BUD \equiv b$ with zero slope; that is,

$$f(R) = \gamma_{max} - a(R - b)^2 \tag{3}$$

is a function with the desired property. (2) It intersects $\gamma = A + B/R$ at some point X, such that

$$\gamma_{max} - a(X - b)^2 = A + B/X \quad . \tag{4}$$

(3) At this point X, the derivatives of the two curves are equal; that is

$$-2a(X - b) = -\frac{B}{X^2} \quad . \tag{5}$$

Combining Eqs. (4) and (5), we get

$$X = \frac{3B + \sqrt{9B^2 - 8(\gamma_{max} - A)bB}}{4(\gamma_{max} - A)} \tag{6}$$

and

$$a = \frac{B}{2X^2(X - b)} \quad . \tag{7}$$

Equation (3) is then used to calculate γ from b to X.

```
      SUBROUTINE PRNT                                                   PRNT      2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM     2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM     3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM     4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                        PARAM     5
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO INIT      2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT      3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)            INIT      4
      COMMON/EOSN/IEOS(ML),ME(ML)                                       EN        2
      COMMON/VOID/INTX(ML2),JV(ML2),IV(ML2),NNV                         VD        2
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                         MCELL     2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)   MCELL     3
     +,W(MCL)                                                           MCELL     4
      LEVEL 2,R                                                         MCELL     5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM, MCELL     6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                    MCELL     7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                  MCELL     8
      LEVEL 2,TIME                                                      MCELL     9
      COMMON/UCJC/UCJ,JJ,NMAX,RCJ,DCJ                                   UC        2
      COMMON/MNMX/KMAX(ML2),KMIN(ML2),NMC                               MN        2
      COMMON/ES/IE(ML2),NME                                             ESM       2
      WRITE(8,4)   TAPE8 = XOUT                                         PRNT     11
    4 FORMAT(1H1)                                                       PRNT     12
      WRITE(8,6)LABEL  Problem label                                    PRNT     13
    6 FORMAT(1X,8A10)                                                   PRNT     14
      WRITE(8,5)TIME,DT,ICYCL  Time (μs), Δt, cycle #                   PRNT     15
    5 FORMAT(//1X,5HTIME=,1PE16.5,1X,4HDT= ,1PE12.5,1X,7HCYCLE= ,I10//) PRNT     16
      PRINT 5,TIME,DT,ICYCL   PRINT → OUTPUT                            PRNT     17
      CALL ESUM  Calculate energy sums                                  PRNT     18
      DO 20 I=1,NME                                                     PRNT     19
      WRITE(8,96)I,EE(I),EE(I+ML),EE(I+2*ML)] Total, kinetic, and internal PRNT  20
      PRINT 96,I,EE(I),EE(I+ML),EE(I+ML*2)  ] energy for each region    PRNT     21
   20 CONTINUE                                                          PRNT     22
      WRITE(8,95)EE(ML),EE(2*ML),EE(3*ML)] Total, kinetic, and internal PRNT     23
      PRINT 95,EE(ML),EE(2*ML),EE(3*ML)  ] energy for the problem       PRNT     24
   95 FORMAT(1X,14H TOTAL ENERGY=,1PE12.5,23H TOTAL INTERNAL ENERGY=,   PRNT     25
     +1PE12.5,22H TOTAL KINETIC ENERGY=,1PE12.5)                        PRNT     26
   96 FORMAT(1X,10H MATERIAL ,I2,8H ENERGY=,1PE12.5,                    PRNT     27
     +17H INTERNAL ENERGY=,1PE12.5,16H KINETIC ENERGY=,1PE12.5)         PRNT     28
      WRITE(8,97)   Cell quantity labels                                PRNT     29
   97 FORMAT(1HO,2X,10HJ IEOS MAT,4X,1HM,10X,1HR,10X,1HV,10X,1HU,10X    PRNT     30
     +,1HI,10X,1HT,10X,1HP,10X,1HQ,9X,2HSX,9X,2HSZ,10X,1HW/)            PRNT     31
      IF(BU.EQ.0.)GO TO 10                                              PRNT     32
      WRITE(8,80)R(1),U(1)   Piston radius and velocity                 PRNT     33
   80 FORMAT(3X,10H1 PISTON  ,10X,2(1PE10.3,12X))                       PRNT     34
      WRITE(8,81)  Region separator                                     PRNT     35
   81 FORMAT(1X,131(1H-))                                               PRNT     36
   10 CONTINUE                                                          PRNT     37
      NMP=NMC                                                           PRNT     38
      IF(ICYCL.EQ.0)NMP=NM   Print all cells for cycle 0                PRNT     39
      DO 11 I=1,NMP  Print all active cells                             PRNT     40
      JMN=JMIN(I)                                                       PRNT     41
      JMX=JMAX(I)                                                       PRNT     42
      IF(ICYCL.EQ.0)JMX=KMAX(I)                                         PRNT     43
      II=IE(I)                                                          PRNT     44
      DO 12 J=JMN,JMX                                                   PRNT     45
      WRITE(8,82)J,IEOS(II),MAT(II),XM(J),R(J),V(J),U(J),XI(J),T(J)     PRNT     46
     +,P(J),Q(J),SX(J),SZ(J),W(J)  Print cell quantities                PRNT     47
   82 FORMAT(1X,2I3,I5,11(1PE10.3,1X))                                  PRNT     48
   12 CONTINUE                                                          PRNT     49
```

```
      JMP=JMX+1                                                          PRNT      50
      IF(II.EQ.IF(I+1))GO TO 13                                          PRNT      51
      WRITE(8,81)  Region separator                                      PRNT      52
      IF(IV(I).NE.-1)WRITE(8,84)JMP,R(JMP),U(JMP)  Radius and velocity at the PRNT 53
      GO TO 14                                      outside of a void ini- PRNT 54
   13 CONTINUE                                      tially in the problem PRNT   55
      WRITE(8,83)  Interface due to spalling                             PRNT      56
   83 FORMAT(1X,131(1H.))                                                PRNT      57
      IF(IV(I).NE.-1)WRITE(8,85)JMP,R(JMP),U(JMP)  Radius and velocity at the PRNT 58
   14 CONTINUE                                      outside of a void due to PRNT 59
   84 FORMAT(1X,I3,5H VOID,2X,2(12X,1PE10.3)/1X,131(1H-))                PRNT      60
   85 FORMAT(1X,I3,5H VOID,2X,2(12X,1PE10.3)/1X,131(1H.))                PRNT      61
   11 CONTINUE                                                           PRNT      62
      IF(NMAX.LT.NCL-1)GO TO 15                                          PRNT      63
      WRITE(8,86)NCL,R(NCL),U(NCL)  Innermost radius and velocity        PRNT      64
   86 FORMAT(1X,I3,7H INSIDE,12X,2(1PE10.3,12X))                         PRNT      65
      NCLP=NCL+1                                                         PRNT      66
      IF(BUI.NE.0.)WRITE(8,87)NCLP,R(NCLP),U(NCLP)  Inside piston        PRNT      67
   87 FORMAT(1X,131(1H-)/1X,I3,7H PISTON,12X,2(1PE10.3,12X))             PRNT      68
   15 CONTINUE                                                           PRNT      69
      WRITE(8,5)TIME,DT,ICYCL                                            PRNT      70
  900 FORMAT(1X,T3,11E11.4)                                              PRNT      71
      RETURN                                                             PRNT      72
      END                                                                PRNT      73
```

PRNT

Makes a cycle printout including time, Δt, cycle #, region and total energies, and cell quantities for active cells.

Local Variables

I = region #.

II = IE(I) = original region #.

J = cell #.

JMN,JMX = JMIN(I),JMAX(I) = minimum and maximum active cell # in a region; for cycle #0, JMX is the maximum cell # in a region.

JMP = JMX+1 = cell # of inside radius of a region.

NCLP = NCL+1 = cell # of the inside piston radius.

NMP = NMC for any cycle # except 0; NMP = NM for cycle #0 so that all cells are printed with their initial conditions.

Notes

The cell quantity lines are longer than 120 characters, so the LONG. option should be used in ALLOUT for printing XOUT or OUTPUT. The dashed region separators are for the original regions in the problem. The dotted region separators are for new regions created by spalling.

```
      SUBROUTINE ESUM                                                    ESUM        2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,          PARAM       2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                   PARAM       3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                     PARAM       4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                         PARAM       5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                          MCELL       2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),TFLAG(MCL)    MCELL       3
     +,W(MCL)                                                            MCELL       4
      LEVEL 2,R                                                          MCELL       5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM,  MCELL       6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                     MCELL       7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                   MCELL       8
      LEVEL 2,TIME                                                       MCELL       9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO  INIT        2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT        3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)             INIT        4
      COMMON/ES/TE(ML2),NME                                              ESM         2
      COMMON/MNMX/KMAX(ML2),KMIN(ML2),NMC                                MN          2
      COMMON/PWORK/PW,PWI                                                PWORK       2
      DATA PI/3.1415926535/                                              ESUM        9
      M3=ML*3                                                            ESUM       10
      GF=PI*IA*2                                                         ESUM       11
      IF(IA.EQ.0)GF=1.   ] Geometry-dependent factor                     ESUM       12
      DO 10 I=1,M3                                                       ESUM       13
   10 EE(I)=0.                                                           ESUM       14
      DO 20 I=1,NM                                                       ESUM       15
      JMN=JMIN(I)                                                        ESUM       16
      JMX=KMAX(I)                                                        ESUM       17
      IT=IE(I)  Original region #; sums are over original regions        ESUM       18
      II=IT+ML                                                           ESUM       19
      IK=II+ML                                                           ESUM       20
      DO 21 J=JMN,JMX                                                    ESUM       21
      EE(II)=XM(J)*XI(J)+EE(II)  Sum of term proportional to internal energy ESUM    22
   21 EE(IK)=XM(J)*(U(J)+U(J+1))**2+EE(IK) Sum of term proportional to    ESUM       23
   20 CONTINUE                                  kinetic energy            ESUM       24
      IJ=IE(NM)                                                          ESUM       25
      DO 23 I=1,IJ                                                       ESUM       26
      II=I+ML                                                            ESUM       27
   23 EE(II)=EE(II)+EE(II+2*ML)  Add energy shift for HE's from HEI(q.v.) ESUM       28
      ITWML=2*ML                                                         ESUM       29
      ITHML=3*ML                                                         ESUM       30
      DO 22 I=1,IJ                                                       ESUM       31
      IML=I+ML                                                           ESUM       32
      ITML=IML+ML                                                        ESUM       33
      EE(IML)=EE(IML)*GF  Scale internal energy to proper value          ESUM       34
      EE(ITML)=EE(ITML)*GF/8  Scale kinetic energy to proper value       ESUM       35
      EE(I)=EE(IML)+EE(ITML)  Total energy for the region                ESUM       36
      EE(ML)=EE(ML)+EE(I)   Total energy for the problem                 ESUM       37
      EE(ITWML)=EE(ITWML)+EE(IML)  Total internal energy for the problem ESUM       38
      EE(ITHML)=EE(ITHML)+EE(ITML)  Total kinetic energy for the problem ESUM       39
   22 CONTINUE                                                           ESUM       40
      IFML=4*ML                                                          ESUM       41
      EE(IFML+1)=GF*PW   ] Scale piston work                             ESUM       42
      EE(IFML+2)=GF*PWI  ]                                               ESUM       43
      EE(ML)=EE(ML)+EE(IFML+1)+EE(IFML+2) Add work done by the pistons to the ESUM   44
      RETURN                                       total energy of the problem ESUM  45
      END                                                                ESUM       46
```

ESUM

Calculates kinetic, internal, and total energies for each region and for the whole problem.

Local Variables

GF = geometry factor = $1, 2\pi, 4\pi$ for $\alpha = 1,2,3$.

I = do loop index (usually region #).

IFML = 4*ML.

II = original region # + ML = index for internal energy.

IJ = original # of regions.

IK = original region # + 2*ML = index for kinetic energy.

IML = same as II.

IT = original region #.

ITML = same as IK.

ITWML = 2*ML = index for total internal energy.

ITHML = 3*ML = index for total kinetic energy.

J = cell #.

JMN,JMX = Minimum and maximum active cell #'s.

M3 = 3*ML.

Notes

The variable EE contains energy sums in cell quantities in the following order:

1 to ML-1	total energy for region 1 to ML-1
ML	total energy for the problem plus work done on pistons
ML+1 to 2*ML-1	internal energy for region 1 to ML-1
2*ML	total internal energy for the problem
2*ML+1 to 3*ML-1	kinetic energy for region 1 to ML-1
3*ML	total kinetic energy for the problem

3*ML+1 to 4*ML-1	shift of the energy zero for HE's so that at infinite expansion of the products, the energy will be zero
4*ML+1	work done on the outside piston
4*ML+2	work done on the inside piston

ML is set in a parameter statement and is usually 21, the number of allowed materials plus one.

The specific internal energy in a cell is in the units Mbar-cm^3/g, which is 10^{12} erg/g. The internal energy in a cell is just the mass of the cell times the specific internal energy. The mass in variable XM is not the actual mass of the cell. For $\alpha = 1$ it is the mass per unit area so that XM(J)*XI(J) is the energy per unit area in cell J. For $\alpha = 2$, XM is the mass per unit length per unit angle. So, 2π*XM(J)*XI(J) is the energy per unit length. For $\alpha = 3$, XM is the mass per unit solid angle. So, 4π*XM(J)*XI(J) is the energy in cell J.

The kinetic energy is calculated from $\frac{1}{2}$ mv^2. For mass in grams and velocity in cm/μs, the unit of kinetic energy is 10^{12} erg = Mbar-cm^3, which agrees with the unit for internal energy. There is also a geometry factor of 1,2π, and 4π of α = 1,2,3, respectively. Also, as above, the energy is per unit area for $\alpha = 1$ and per unit length for $\alpha = 2$. A cell-centered velocity is used to calculate the kinetic energy in a cell.

The energies for a region are calculated for the original region even if it is later split into more than one region. For HE's, the internal energy has a constant added so that the energy zero is shifted to that of the products expanded to infinite volume. For the total energy of the problem, the work done on pistons is also included so that the total energy should be constant to a good approximation.

```
      SUBROUTINE WDUMP                                                  WDUMP     2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM     2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM     3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM     4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                        PARAM     5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                         MCELL     2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)   MCELL     3
     +,W(MCL)                                                           MCELL     4
      LEVEL 2,R                                                         MCELL     5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM, MCELL     6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                    MCELL     7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                  MCELL     8
      LEVEL 2,TIME                                                      MCELL     9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO  INIT      2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT      3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QQ(ML),TMLT(ML),TMC(ML)            INIT      4
      COMMON/USUPC/C1(ML),S1(ML),C2(ML),S2(ML),SWV(ML),VMN(ML),         US        2
     +GAMMA(ML),ALP(ML)                                                 US        3
      COMMON/BRND/Z(ML),E(ML),VCJ(ML),DWDT(NDW,ML),PCJ(ML),PM(ML),ND(ML) BRD      2
     +,MSFF                                                             BRD       3
      COMMON/GASC/GC(NGC,ML)                                            GC        2
      COMMON/FGHIJC/FS(ML),GS(ML),HS(ML),SI(ML),SJ(ML),CV(ML)           FG        2
      COMMON/UCJC/UCJ,JJ,NMAX,RCJ,DCJ                                   UC        2
      COMMON/VOID/INTX(ML2),JV(ML2),IV(ML2),NNV                         VD        2
      COMMON/MNMX/KMAX(ML2),KMIN(ML2),NMC                               MN        2
      COMMON/BRNS/A(ML),BR(ML),BA(ML),VBO(ML),VBSW(ML)                  BRN       2
      COMMON/EOSN/IEOS(ML),ME(ML)                                       EN        2
      COMMON/NSPLT/NOSPLT(ML2)                                          NSP       2
      COMMON/SPC/SP(ML),USP(ML)                                         SPLC      2
     +,XISP(ML)                                                         SPLC      3
      COMMON/POLYC/CF(NCF,ML),PS(ML)                                    PLC       2
      COMMON/GAS/FI(1003),DI(MQL)                                       GS        2
      LEVEL 2,FI                                                        GS        3
      COMMON/LEV/DMPNO                                                  GS        4
      LEVEL 2,DMPNO                                                     GS        5
      COMMON/BUX/BUA,BUB,BUMAX,BUDV(ML)                                 BUP       2
     +,BUR,BUD                                                          BUP       3
      COMMON/RLC/RC(ML),RP(ML),RLV(ML),PH1,DV1,DV2                      RLC       2
      DIMENSION XINDX(NDX),INDX(NDX)                                    WDUMP    21
      EQUIVALENCE (XINDX(1),INDX(1))                                    WDUMP    22
      DATA IST/1/                                                       WDUMP    23
      IF(IST.NE.1)GO TO 2   Initialize                                  WDUMP    24
      IST=2                                                             WDUMP    25
      I=1                                                               WDUMP    26
      J=0                                                               WDUMP    27
      L1=LOCF(DV2)-LOCF(NDF)+1   SCM length                             WDUMP    28
      L2=LOCF(JS)-LOCF(R(1))+1   LCM length                             WDUMP    29
      L12=L1+L2  Total length per dump                                  WDUMP    30
      LEN=(L12+2)*MXDUMP+2  Total length of file to allow MXDUMP restart dumps  WDUMP  31
      INDX(1)=L12                                                       WDUMP    32
      INDX(2)=0                                                         WDUMP    33
      CALL QASSIGN(1,5HDUMP0,0,0)   ]                                   WDUMP    34
      CALL FAMSIZ(1,LEN)            ]  Set up DUMP0 file                WDUMP    35
      CALL FAMWAIT(1,1)             ]                                   WDUMP    36
    2 CONTINUE                                                          WDUMP    37
      J=J+1                 ]                                         WDUMP    38
      INDX(2)=J             ]  The index has the form:                  WDUMP    39
      I=I+2                 ]  L12, last dump #, cycle1, time1, ···, cycle_MXDUMP,  WDUMP  40
      INDX(I)=ICYCL         ]  time_MXDUMP                              WDUMP    41
      XINDX(I+1)=TIME       ]                                           WDUMP    42
```

```
      CALL WDISK(1,XINDX,NDX,0)  Write the index                          WDUMP      43
      IF(UNIT(1))10,10,10                                                 WDUMP      44
   10 CONTINUE                                                            WDUMP      45
      N1=NDX+L12*(J-1)]  Find the locations for the SCM and LCM dumps     WDUMP      46
      N2=N1+L1         ]                                                  WDUMP      47
      CALL WDISK(1,NDF,L1,N1)  Write the SCM dump                         WDUMP      48
      IF(UNIT(1))11,11,11                                                 WDUMP      49
   11 CONTINUE                                                            WDUMP      50
      CALL WDISK(1,F,L2,N2)  Write the LCM dump                           WDUMP      51
      IF(UNIT(1))12,12,12                                                 WDUMP      52
   12 CONTINUE                                                            WDUMP      53
      PRINT 100,J,ICYCL,TIME                                              WDUMP      54
  100 FORMAT(1X,4HDUMP,I4,9H AT CYCLE,I10,6H,TIME=,E12.5)                 WDUMP      55
      IF(J.LT.MXDUMP)RETURN                                               WDUMP      56
      PRINT 101                                                           WDUMP      57
      WRITE(9,101)                ] If this is the last allowed dump, STOP WDUMP      58
  101 FORMAT(16H LAST DUMP: STOP)]                                        WDUMP      59
      STOP                                                                WDUMP      60
      END                                                                 WDUMP      61
```

WDUMP

Writes a restart dump (all of the necessary data to restart the problem at a given cycle). (Inactive regions may be replaced with new setup information so that two different problems that start out the same may be restarted at a time before they differ without completely rerunning the problem.)

Local Variables

I = location in the index where the cycle # at this dump is stored = 2*J.

J = dump #.

L1 = # of words in SCM to be dumped.

L2 = # of words in LCM to be dumped.

L12 = L1 + L2.

LEN = total length of the dump file required to make MXDUMP dumps.

N1 = starting location for writing the SCM data.

N2 = starting location for writing the LCM data.

Notes

All of the variables to be dumped are in common blocks. The order in which they are stored in memory is specified by the order they appear in MAIN. The SCM and LCM data are separated so they are dumped separately. The number of words of SCM and LCM data are each determined by using the standard function LOCF (which returns the address for a given variable) to get the location of the first variable in the first common block and the last variable in the last common block to be dumped. The index is written in the following order beginning with word 0 of the dump file: L12, last dump #, 1st cycle #, 1st time, 2nd cycle #, 2nd time, ···, last cycle #, last time. If the last allowed dump (MXDUMP is usually 30) is made, the problem is stopped.

```
      SUBROUTINE RDUMP(I)                                                RDUMP      2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,          PARAM      2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                   PARAM      3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                     PARAM      4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                         PARAM      5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                          MCELL      2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)    MCELL      3
     +,W(MCL)                                                            MCELL      4
      LEVEL 2,R                                                          MCELL      5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM,  MCELL      6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                     MCELL      7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                   MCELL      8
      LEVEL 2,TIME                                                       MCELL      9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO  INIT       2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT       3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)             INIT       4
      COMMON/USUPC/C1(ML),S1(ML),C2(ML),S2(ML),SWV(ML),VMN(ML),          US         2
     +GAMMA(ML),ALP(ML)                                                  US         3
      COMMON/BRND/Z(ML),E(ML),VCJ(ML),DWDT(NDW,ML),PCJ(ML),PM(ML),ND(ML) BRD        2
     +,MSFF                                                              BRD        3
      COMMON/GASC/GC(NGC,ML)                                             GC         2
      COMMON/FGHIJC/FS(ML),GS(ML),HS(ML),SI(ML),SJ(ML),CV(ML)            FG         2
      COMMON/UCJC/UCJ,JJ,NMAX,RCJ,DCJ                                    UC         2
      COMMON/VOID/INTX(ML2),JV(ML2),IV(ML2),NNV                          VD         2
      COMMON/MNMX/KMAX(ML2),KMIN(ML2),NMC                                MN         2
      COMMON/BRNS/A(ML),BR(ML),BA(ML),VBO(ML),VBSW(ML)                   BRN        2
      COMMON/EOSN/TEOS(ML),ME(ML)                                        EN         2
      COMMON/NSPLT/NOSPLT(ML2)                                           NSP        2
      COMMON/SPC/SP(ML),USP(ML)                                          SPLC       2
     +,XISP(ML)                                                          SPLC       3
      COMMON/POLYC/CF(NCF,ML),PS(ML)                                     PLC        2
      COMMON/GAS/FI(1003),DI(MQL)                                        GS         2
      LEVEL 2,FI                                                         GS         3
      COMMON/LEV/DMPNO                                                   GS         4
      LEVEL 2,DMPNO                                                      GS         5
      COMMON/BUX/BUA,BUB,BUMAX,BUDV(ML)                                  BUP        2
     +,BUR,BUD                                                           BUP        3
      COMMON/RLC/RC(ML),RP(ML),RLV(ML),PH1,DV1,DV2                       RLC        2
      DIMENSION L(2)                                                     RDUMP     21
      CALL QASSIGN(2,5HDUMPI,0,0)  Restart dump read from file DUMPI     RDUMP     22
      CALL RDISK(2,L,2,0)    Read the first two words of the index       RDUMP     23
      IF(UNIT(2))10,10,10                                                RDUMP     24
   10 CONTINUE                                                           RDUMP     25
      IF(L(2).LT.I)GO TO 991   Are there I dumps                         RDUMP     26
      L1=LOCF(DV2)-LOCF(NDF)+1   SCM length                              RDUMP     27
      L2=LOCF(JS)-LOCF(R(1))+1   LCM length                              RDUMP     28
      L12=L1+L2  Total length                                            RDUMP     29
      N1=NDX+L12*(I-1)  SCM address                                      RDUMP     30
      N2=N1+L1    LCM address                                            RDUMP     31
      IF(L12.NE.L(1))GO TO 992  If L12 ≠ L(1), then dimensions don't match RDUMP   32
      CALL RDISK(2,NDF,L1,N1)  Read SCM variables                        RDUMP     33
      IF(UNIT(2))11,11,11                                                RDUMP     34
   11 CONTINUE                                                           RDUMP     35
      CALL RDISK(2,R,L2,N2)  Read LCM variables                          RDUMP     36
      IF(UNIT(2))12,12,12                                                RDUMP     37
   12 CONTINUE                                                           RDUMP     38
      RETURN                                                             RDUMP     39
  991 CONTINUE                                                           RDUMP     40
      PRINT 101,I                                                        RDUMP     41
  101 FORMAT(5H DUMP,I5,21H DOES NOT EXIST: STOP)                        RDUMP     42
```

```
      WRITE(9,101)I                                                    RDUMP     43
      GO TO 999                                                        RDUMP     44
  992 CONTINUE                                                         RDUMP     45
      PRINT 102    In this case check for differences in the parameter statement  RDUMP     46
      WRITE(9,102)  or for any changes in any common block             RDUMP     47
  102 FORMAT(33H DUMP LENGTH DOES NOT MATCH: STOP)                     RDUMP     48
  999 CONTINUE                                                         RDUMP     49
      STOP                                                             RDUMP     50
      END                                                              RDUMP     51
```

RDUMP

Reads the restart dump and stores all of the data in the appropriate locations.

Local Variables

L = array containing the 1st two words of the dump index in the file DUMPI (see WDUMP).

L1 = # of words in SCM that should be read.

L2 = # of words in LCM that should be read.

L12 = L1 + L2, which = L(1) for a valid restart.

N1 = first word address for the SCM part of the dump to be read.

N2 = first word address for the LCM part of the dump to be read.

Notes

If L12 $\neq$ L(1), then the number of words in the dump does not match the variables into which the data is to be stored. Then either the code has been changed incorrectly between the two runs or one of the array sizes in the PARAMETER statement has been changed. In either case, the code would not run properly and is terminated.

```
      SUBROUTINE OUTGAS                                                 OUTGAS     2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM      2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM      3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM      4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                        PARAM      5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                         MCELL      2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)   MCELL      3
     +,W(MCL)                                                           MCELL      4
      LEVEL 2,R                                                         MCELL      5
      COMMON/OVL/NDE,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM, MCELL      6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                    MCELL      7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                  MCELL      8
      LEVEL 2,TIME                                                      MCELL      9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO INIT       2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT      3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)            INIT       4
      COMMON/GAS/FI(1003),DI(MQL)                                       GS         2
      LEVEL 2,FI                                                        GS         3
      COMMON/LEV/DMPNO                                                  GS         4
      LEVEL 2,DMPNO                                                     GS         5
      COMMON/MNMX/KMAX(ML2),KMIN(ML2),NMC                               MN         2
      COMMON/VOID/INTX(ML2),JV(ML2),IV(ML2),NNV                         VD         2
      COMMON/ES/IE(ML2),NME                                             ESM        2
      DIMENSION DATIN(MCL,NUMV)                                         OUTGAS    10
      EQUIVALENCE (DATIN,R)                                             OUTGAS    11
      DIMENSION IFI(1003),IDI(MQL)                                      OUTGAS    12
      EQUIVALENCE (FI,IFI),(DI,IDI)                                     OUTGAS    13
      DIMENSION TTMP(100)                                               OUTGAS    14
      DATA (ISTFLAG=1)                                                  OUTGAS    15
      DATA IBLANK/10H                                                   OUTGAS    16
      DATA IMC/5/                                                       OUTGAS    17
      GO TO (1,2),ISTFLAG        Initialize                             OUTGAS    18
    1 ISTFLAG=2                                                         OUTGAS    19
      IFI(1)=1003                                                       OUTGAS    20
      IFI(2)=0                                                          OUTGAS    21
      IFI(3)=1003                                                       OUTGAS    22
      NUMVP=NUMV+2   Total # of variables including region flag and time OUTGAS    23
C                                                                       OUTGAS    24
C      THIS CODE WRITES A RANDOM M2C FILE                               OUTGAS    25
C         NO CONVERSION IS NECESSARY IN GAS                             OUTGAS    26
C                                                                       OUTGAS    27
C      COMPUTE THE # OF PACKED WORDS PER CELL                           OUTGAS    28
      NWPC=(NUMVP-1)/3+1   # of packed words per cell                   OUTGAS    29
      NAF=2                                                             OUTGAS    30
      NA=3                                                              OUTGAS    31
      IF(IJK.LE.0)IJK=1    Use every IJKth cell                         OUTGAS    32
      NCLP=NCL+55   Allow 55 extra cells from splits and spalls         OUTGAS    33
      IF(NCLP.GE.MCL) NCLP=MCL-1   Don't allow for more than dimensioned OUTGAS    34
      NVN=100+NWPC*((NCLP+IJK-1)/IJK)  # words per dump                 OUTGAS    35
      LENGTH=500*NVN+1003+512  Total # of words needed for 500 dumps    OUTGAS    36
      CALL FAMST7(3,LENGTH)   Make GASSIN that length                   OUTGAS    37
      CALL FAMWAIT(3,1)                                                 OUTGAS    38
C     THE MAGIC FIRST HUNDRED WORDS                                     OUTGAS    39
      IDI(3)=1                                                          OUTGAS    40
      IDI(5)=NWPC  # words per cell                                     OUTGAS    41
      IDI(6)=3    # variables per word                                  OUTGAS    42
      IDI(10)=14  # of fraction bits in packed word                     OUTGAS    43
      IDI(11)=5   # of exponent bits in packed word                     OUTGAS    44
      CALL DATE4(IDATE)  ] Get the date and put it on graphs            OUTGAS    45
      IDI(81)=IDATE      ]                                              OUTGAS    46
```

```
      IDI(82)=IBLANK]  Label is currently blank                          OUTGAS     47
      IDI(83)=IBLANK]                                                   OUTGAS     48
      IDI(90)=LABEL(1)]                                                 OUTGAS     49
      IDI(91)=LABEL(2)  Put the 1st 30 characters of LABEL in           OUTGAS     50
      IDI(92)=LABEL(3)]  the classification words                       OUTGAS     51
      IDI(93)=1                                                         OUTGAS     52
      IDI(94)=1                                                         OUTGAS     53
    2 CONTINUE                                                          OUTGAS     54
      IF(IFI(2).GE.500) RETURN                                          OUTGAS     55
C                                                                       OUTGAS     56
      DO 10 I=1,NMC                                                     OUTGAS     57
      J=JV(I)                                                           OUTGAS     58
      IF(IV(I))10,11,12                                                 OUTGAS     59
   11 P(J)=0.]                                                          OUTGAS     60
      Q(J)=0.                                                           OUTGAS     61
      SX(J)=0.                                                          OUTGAS     62
      SZ(J)=0.   Set cell quantities to 0 in the void cell for open voids OUTGAS     63
      W(J)=0.                                                           OUTGAS     64
      V(J)=0.                                                           OUTGAS     65
      XI(J)=0.]                                                         OUTGAS     66
      GO TO 10                                                          OUTGAS     67
   12 P(J)=(P(J+1)+P(J-1))/2]                                           OUTGAS     68
      Q(J)=(Q(J+1)+Q(J-1))/2                                            OUTGAS     69
      SX(J)=(SX(J+1)+SX(J-1))/2                                         OUTGAS     70
      SZ(J)=(SZ(J+1)+SZ(J-1))/2  Interpolate cell quantities for a closed void OUTGAS  71
      W(J)=(W(J+1)+W(J-1))/2                                            OUTGAS     72
      V(J)=(V(J+1)+V(J-1))/2                                            OUTGAS     73
      XI(J)=(XI(J+1)+XI(J-1))/2]                                        OUTGAS     74
   10 CONTINUE                                                          OUTGAS     75
      CALL ESUM  Calculate energy sums                                  OUTGAS     76
      DMPNO=TIME                                                        OUTGAS     77
      ITMP(2)=ICONV(DMPNO)  2nd variable is time                        OUTGAS     78
      NA=NA+2                                                           OUTGAS     79
      DI(1)=DMPNO   Dump # is time                                      OUTGAS     80
      IDI(2)=NCLP                                                       OUTGAS     81
C     FILE INDEX                                                        OUTGAS     82
      NAF=NAF+2   # words in file index                                 OUTGAS     83
      FI(NAF)=DMPNO  time word                                          OUTGAS     84
      IFI(NA)=IFT(3)+1  FWA of dump                                     OUTGAS     85
      IFI(2)=IFI(2)+1   # of dumps                                      OUTGAS     86
      IFI(3)=IFI(3)+NVN  Last word address of dump                      OUTGAS     87
C   WRITE OUT TO DISK THE FIRST 1003 WORDS: FILE INDEX                  OUTGAS     88
      CALL WDISK(3,FI,1003,0)                                           OUTGAS     89
      IF(UNIT(3)) 152,152,152                                           OUTGAS     90
  152 CONTINUE                                                          OUTGAS     91
C      PACK 'EM                                                         OUTGAS     92
      IIA=100                                                           OUTGAS     93
      I=1                                                               OUTGAS     94
      DO 210 L=1,NCL,IJK                                                OUTGAS     95
      IF(L.GT.KMAX(I))I=I+1                                             OUTGAS     96
      ITMP(1)=IFLAG(L)/64  1st variable is a region #                   OUTGAS     97
C      SHIFT 'EM TO 20 BIT WORDS                                        OUTGAS     98
      DO 220 K=3,NUMVP                                                  OUTGAS     99
  220 ITMP(K)=ICONV(DATIN(L,K-2))  Convert to 20-bit words              OUTGAS    100
      II=IE(I)                                                          OUTGAS    101
      IF(XMU(II).EQ.0.)ITMP(9)=ICONV(W(L))  Store W in SZ's place if μ = 0 OUTGAS 102
      DO 230 K=1,NUMVP,3                                                OUTGAS    103
      IIA=IIA+1                                                         OUTGAS    104
  230 DI(IIA)=SHIFT(ITMP(K),40).OR.SHIFT(ITMP(K+1),20).OR.ITMP(K+2)     OUTGAS    105
  210 CONTINUE  Put three 20-bit words together to make one 60-bit word OUTGAS    106
```

```
      IF(IIA.GE.NVN) GO TO 400
      IO=IIA-NWPC+1
      IP=IIA+1                          Fill unused cells with data
      DO 300 L=IP,NVN                    from the last cell used
      DI(L)=DI(IO)
      IO=IO+1
  300 CONTINUE
  400 CONTINUE
C     WRITE OUT TO DISK THE DATA
      CALL WDISK(3,DT,NVN,IFI(NA))
      IF(UNIT(3)) 340,340,340
  340 CONTINUE
      RETURN
      END
```

OUTGAS 107
OUTGAS 108
OUTGAS 109
OUTGAS 110
OUTGAS 111
OUTGAS 112
OUTGAS 113
OUTGAS 114
OUTGAS 115
OUTGAS 116
OUTGAS 117
OUTGAS 118
OUTGAS 119
OUTGAS 120

OUTGAS

Makes a GAS dump to file GASSIN which includes most cell quantities. GASSIN may be postprocessed to give on the Tektronix/film/fiche any cell variable as a function of any other cell variable (e.g., pressure vs radius) at a given time, time plot a cell variable for a given cell, r-t plots of interfaces, cell positions for each cell, contour plots of a cell variable in r-t space, etc.

Local Variables

IBLANK = 10 blank Hollerith characters used in the plot label.

IDI = array containing the first 100 words in each dump.

IFI = array containing the first 1003 words of GASSIN which contains the file index.

IIA = counter to keep track of the index for DI.

IJK = only dump every IJKth cell (usually IJK = 1).

IO, IP } indices used to copy the packed data for the last cell into the remaining space for a data dump.

ISTFLAG = flag that is 1 for the 1st time through and 2 otherwise.

ITMP = array to contain the 20-bit words before they are combined 3 to a word.

J = cell # for voids.

K = do loop index.

L = do loop index.

LENGTH = length of the file GASSIN that will hold 500 dumps.

NA = index to give the location in IFI that the 1st word address for the current dump is stored.

NAF = NA+1 = index to give the location in IFI that the dump time for the current dump is stored.

NCLP = # of cells allowed per dump = initial NCL plus 55 to allow for rezoning and spalling.

NUMVP = # of variables stored per cell.

NVN = # of words per dump.

NWPC = # of words per cell.

Notes

The cell variables are stored with the following variable numbers.

1 = region index

2 = time

3 = radius

4 = velocity

5 = specific internal energy

6 = specific volume

7 = pressure

8 = stress deviator in the X direction

9 = stress deviator in the Z direction or mass fraction if $\mu = 0$

10 = energy sums (see ESUM)

11 = temperature

12 = viscosity

Space is provided for 55 extra cells to be added due to space splits and/or spalling. Data from the last word is repeated in the unused cells. This is to allow the new cells added to also be plotted. The repetition of the last cell data is necessary for two-dimensional and r-t plots of all cells to avoid extraneous lines. Details of the GAS file and how to run GAS are given in LTSS-523.

```
      FUNCTION ICONV(X)                                                  ICONV     2
      LEVEL 2,X                                                          ICONV     3
C     FORM A 20 BIT FLOATING POINT WORD FOR MAGEE MOVIE                  ICONV     4
      DATA IFA/1700000008/,IFB/37777778/,IFC/37777768/                   ICONV     5
      ISIGN=0                                                            ICONV     6
      IF(X.LT.0.) ISIGN=1                                                ICONV     7
      JS=SHIFT(ABS(X),-33)-IFA                                           ICONV     8
      IF(JS.GT.IFB) JS=IFB    Maximum allowed value of JS                ICONV     9
      IF(JS.LT.0) JS=0    Minimum allowed value of JS                    ICONV    10
      ICONV=(JS.AND.IFC).OR.ISIGN  20-bit word with sign in bit 0        ICONV    11
      RETURN                                                             ICONV    12
      END                                                                ICONV    13
```

ICONV(X)

Takes a 60-bit floating point word and converts it to a 20-bit floating point word.

Local Variables

IFA = bit pattern to shift the bias of the exponent.

IFB = maximum allowed integer value of the 20-bit word = 20 bits of 1's.

IFC = the 19 bits for exponent and integer coefficient are 1's.

ISIGN = the sign of X.

JS = the 20-bit word before the sign bit is set correctly.

Notes

The 60-bit floating point word has the following structure:

1 sign bit at bit #59.

11 exponent bits at bits 48-58, with a bias of 2000B.

48 integer coefficient bits at bits 0-47.

The desired 20-bit floating point structure is as follows:

5 exponent bits at bits 15-19, with a bias of 100B.

14 integer coefficient bits at bits 1-14.

1 sign bit at bit #0.

The 20-bit word has about 4 significant figures. Negative numbers are stored in 1's complement form for the 60-bit word but not for the 20-bit word. The sign of X is stored in ISIGN. The absolute value of X is then shifted to the right 33 bits and IFA is subtracted from this value to give JS. This puts the exponent bits at 15-25 and the integer coefficient bits at 0-14. Subtracting IFA shifts the exponent bias from 2000B to 100B. By using only 14 bits of the integer coefficient, there is also an effective shift of 34 bits or 42B. If JS > IFB, then a 5-bit exponent is not sufficient and the maximum allowed 20-bit word is used. If JS < 0, then the exponent is too small and a

value of 0 is used. Then the 0 bit is set with the sign bit and the 20-bit word conversion is complete. Bits 20-59 are all 0. The largest 20-bit word is 2777776B which is $2^{16} - 2 = 65534$. The smallest positive 20-bit word is 0060000B which is $2^{-16} \doteq 1.5 * 10^{-5}$.

An an exercise, the interested reader can follow the conversion of a floating point 1.0 from the 60-bit octal work 17204 00000 00000 00000 B to the 20-bit octal word 2040000B.

```
      SUBROUTINE DIFEQ                                                  DIFEQ      2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM      2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM      3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM      4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                        PARAM      5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                         MCELL      2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)   MCELL      3
     +,W(MCL)                                                           MCELL      4
      LEVEL 2,R                                                         MCELL      5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM, MCELL      6
     +IALPH,NDELT,LABFL(8),NDUMP,IDMP,NM1,TD(ML),IJK                    MCELL      7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                  MCELL      8
      LEVEL 2,TIME                                                      MCELL      9
      GO TO (1,2),NDF  Index to determine type of differencing scheme   DIFEQ      5
    1 CALL HYDRO   HYDROX                                               DIFEQ      6
      RETURN                                                            DIFEQ      7
    2 CALL SINX   SIN                                                   DIFEQ      8
      RETURN                                                            DIFEQ      9
      END                                                               DIFEQ     10
```

DIFEQ

Switching routine to determine the type of difference equation scheme to be used in the main hydro cycle. Default is HYDRO.

Notes

NDF	Type of Difference Equations
1	Hydrox (see HYDRO)
2	SIN (see SINX)

Any other type of differencing scheme may be added by extending the computed go to statement list and adding the subroutine call and the subroutine.

```
      SUBROUTINE HYDRO                                                    HYDRO     2
C                                                                         HYDRO     3
C     PERFORMS THE BASIC HYDRONAMICS CYCLE                                HYDRO     4
C     CHANGES IN THE DIFFERENCE EQUATIONS MAY BE MADE                     HYDRO     5
C     EXCLUSIVELY IN THIS SUBROUTINE                                      HYDRO     6
C                                                                         HYDRO     7
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,           PARAM     2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                    PARAM     3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                      PARAM     4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                          PARAM     5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                           MCELL     2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)     MCELL     3
     +,W(MCL)                                                             MCELL     4
      LEVEL 2,R                                                           MCELL     5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM,   MCELL     6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                      MCELL     7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                    MCELL     8
      LEVEL 2,TIME                                                        MCELL     9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO   INIT      2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),I8RN(ML),PLAP(ML),DRO(ML),  INIT      3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)              INIT      4
      COMMON/UCJC/UCJ,JJ,NMAX,RCJ,DCJ                                     UC        2
      COMMON/MNMX/KMAX(ML2),KMIN(ML2),NMC                                 MN        2
      COMMON/EOSN/IEOS(ML),ME(ML)                                         EN        2
      COMMON/VOID/INTX(ML2),JV(ML2),IV(ML2),NNV                           VD        2
      COMMON/ES/IE(ML2),NME                                               ESM       2
R^(α-1)dσ/dM DSDM(J,JM)=2*R(J)**IA*(P(JM)+Q(JM)-P(J)-Q(J))/(XM(J)+XM(JM))  HYDRO    16
(α-1)Vφ/R VFR(J,JM)=IA*(V(J)+V(JM))*(2*(SX(J)+SX(JM))+SZ(J)+SZ(JM))/(4*R(J)) HYDRO  17
       φ PH(J,JM)=2*SX(J)+SZ(J)+XM(J)*(2*(SX(J)-SX(JM))-SZ(J)+SZ(JM))/    HYDRO     18
     1 (XM(J)+XM(JM))                                                     HYDRO     19
      VV(J,JM)=V(J)+XM(J)*(V(J)-V(JM))/(XM(J)+XM(JM)) V                   HYDRO     20
      DO 10 I=1,NMC                                                       HYDRO     21
      JMN=JMIN(I)                                                         HYDRO     22
      JMX=JMAX(I)                                                         HYDRO     23
      DO 10 J=JMN,JMX                                                     HYDRO     24
      XI(J)=XI(J)-V(J)*DT*0.5*((P(J)+Q(J))*(U(J+1)-U(J))/                 HYDRO     25
     1  (R(J+1)-R(J))+IA*(P(J)+Q(J)-2*SX(J)-SZ(J))*(U(J+1)+U(J))/         HYDRO     26
     2  (R(J+1)+R(J)))  Part of ΔI that uses old R,V,U                    HYDRO     27
10    CONTINUE                                                            HYDRO     28
      DO 20 I=1,NMC                                                       HYDRO     29
      JMN=JMIN(I)                                                         HYDRO     30
      JMX=JMAX(I)                                                         HYDRO     31
      IF(I.NE.1)JMN=JMN+1                                                 HYDRO     32
      IF(JMN.GT.JMX)GO TO 20                                              HYDRO     33
      DO 21 J=JMN,JMX                                                     HYDRO     34
      JM=J-1                                                              HYDRO     35
      U(J)=U(J)-DT*DSDM(J,JM)                                             HYDRO     36
      IF(INTX(I).GT.2) U(J)=U(J)-DT*VFR(J,JM)   ∂u/∂t = -R^(α-1) ∂σ/∂M - (α-1) Vφ/R   HYDRO 37
      R(J)=R(J)+DT*U(J)  ∂R/∂t = u                                        HYDRO     38
21    CONTINUE                                                            HYDRO     39
      IF(JMAX(I).NE.KMAX(I))GO TO 20                                      HYDRO     40
      IF(I.EQ.NMC.AND.NMC.NE.NM)GO TO 20                                  HYDRO     41
      IF(IV(I))31,32,33  Treat interface as a special case                HYDRO     42
31    J=JMX+1    No artificial void cell                                  HYDRO     43
      GO TO 22                                                            HYDRO     44
32    J=JMX+1                                                             HYDRO     45
      JP=J+1                                                              HYDRO     46
      U(J)=U(J)-DT*2*R(J)**IA*(P(JMX)+Q(JMX))/XM(JMX)   Open void:        HYDRO     47
      R(J)=R(J)+DT*U(J)                                 free surfaces     HYDRO     48
      U(JP)=U(JP)+DT*2*R(JP)**IA*(P(JP)+Q(JP))/XM(JP)                     HYDRO     49
```

```
      R(JP)=R(JP)+DT*U(JP)                                                  HYDRO      50
      GO TO 20                                                              HYDRO      51
33    J=JMX+2    Closed void                                                HYDRO      52
22    CONTINUE                                                              HYDRO      53
      GO TO (1,2,3,4,5),INTX(I)  Boundary conditions depend on μ's          HYDRO      54
5     U(J)=U(J)-DT*VFR(J,JMX)                                               HYDRO      55
1     U(J)=U(J)-DT*DSDM(J,JMX)                                              HYDRO      56
      R(J)=R(J)+DT*U(J)                                                     HYDRO      57
      IF(IV(I).EQ.-1)GO TO 20                                               HYDRO      58
      U(J-1)=U(J)                                                           HYDRO      59
      R(J-1)=R(J)                                                           HYDRO      60
      GO TO 20                                                              HYDRO      61
3     D=IA*(PH(JMX,JMX-1)*VV(JMX,JMX-1)*XM(JMX)/(XM(J)                      HYDRO      62
     1 +XM(JMX)))/R(J)                                                      HYDRO      63
      GO TO 6                                                               HYDRO      64
2     D=IA*PH(J,J+1)*VV(J,J+1)*XM(J)/((XM(J)+XM(JMX))*R(J))                 HYDRO      65
      GO TO 6                                                               HYDRO      66
4     FM=XM(J)/(XM(J)+XM(JMX))                                              HYDRO      67
      D=IA*(PH(J,J+1)*VV(J,J+1)*FM+PH(JMX,JMX-1)*VV(JMX,JMX-1)*(1-FM))      HYDRO      68
     1 /R(J)                                                                HYDRO      69
6     U(J)=U(J)-DT*(D+DSDM(J,JMX))                                          HYDRO      70
      R(J)=R(J)+U(J)*DT                                                     HYDRO      71
      IF(IV(I).EQ.-1)GO TO 20                                               HYDRO      72
      U(J-1)=U(J)                                                           HYDRO      73
      R(J-1)=R(J)                                                           HYDRO      74
20    CONTINUE                                                              HYDRO      75
      CALL BNDR1   Check other boundary conditions                          HYDRO      76
      MR=1                                                                  HYDRO      77
      MRP=1                                                                 HYDRO      78
      DO 30 I=1,NMC                                                         HYDRO      79
      JMN=JMIN(I)                                                           HYDRO      80
      JMX=JMAX(I)                                                           HYDRO      81
      II=IE(I)                                                              HYDRO      82
      DO 30 J=JMN,JMX                                                       HYDRO      83
      MRM=MR                                                                HYDRO      84
      MR=MRP                                                                HYDRO      85
      MRP=IFLAG(J+1)/64    New volume                                       HYDRO      86
      V(J)=F2*(R(J)-R(J+1))*(R(J)**IA+R(J+1)**IA+F3*R(J)*R(J+1))/XM(J)      HYDRO      87
      XI(J)=XI(J)-V(J)*DT*0.5*((P(J)+Q(J))*(U(J+1)-U(J))/                   HYDRO      88
     1  (R(J+1)-R(J))+IA*(P(J)+Q(J)-2*SX(J)-SZ(J))*(U(J+1)+U(J))/           HYDRO      89
     2  (R(J+1)+R(J)))      Part of ΔI that uses new R,V,U                  HYDRO      90
      IF(XMU(II).EQ.0.)GO TO 12                                             HYDRO      91
      SX(J)=SX(J)-4*XMU(II)*DT*((U(J+1)-U(J))/(R(J+1)-R(J))                 HYDRO      92
     1  -IA*0.5*(U(J+1)+U(J))/(R(J+1)+R(J)))/3                              HYDRO      93
      IF(IALPH.EQ.2)GO TO 13                                                HYDRO      94
      SZ(J)=-SX(J)/2              New Stress deviators                      HYDRO      95
      GO TO 12                                                              HYDRO      96
13    SZ(J)=SZ(J)+2*XMU(II)*DT*((U(J+1)-U(J))/(R(J+1)-R(J))                 HYDRO      97
     1  +(U(J+1)+U(J))/(R(J+1)+R(J)))/3                                     HYDRO      98
12    CONTINUE                                                              HYDRO      99
C     XI(J)=XI(J)+DT*((XL(MR)+XL(MRP)))*(T(J+1)-T(J))*R(J+1)**IA/(R(J+2)    HYDRO     100
C     1  -R(J))-(XL(MR)+XL(MRM))*(T(J)-T(J-1))*R(J)**IA/(R(J+1)-R(J-2))     HYDRO     101
C     2  )/XM(J)                                                            HYDRO     102
30    CONTINUE                                                              HYDRO     103
      CALL VISC   New Q's                                                   HYDRO     104
      DO 60 I=1,NMC                                                         HYDRO     105
      II=IE(I)                                                              HYDRO     106
60    IF(IBRN(II).GT.0)CALL BURN(I)  New W's                                HYDRO     107
      CALL EOS  New P's and T's                                             HYDRO     108
      DO 80 I=1,NM                                                          HYDRO     109
```

```
      II=IE(I)                                                          HYDRO    110
      JMN=JMIN(I)                                                       HYDRO    111
      JMX=JMAX(I)                                                       HYDRO    112
      IF(IV(I).EQ.2)CALL RLEOS(I)  Special for high-yelocity impact     HYDRO    113
   80 CONTINUE                                                          HYDRO    114
      CALL BNDR2  More boundary conditions (an entry point in BNDR1)    HYDRO    115
      RETURN                                                            HYDRO    116
      END                                                               HYDRO    117
```

HYDRO

The main hydro cycle using the HYDROX difference equations. New values of radii, velocities, specific volumes, specific internal energies, and stress deviators are calculated. Subroutines are called to get new pressures, temperatures, and artificial viscosities.

Statement Functions

DSDM(J,JM) = difference form of $R^{\alpha-1}\frac{\partial\sigma}{\partial M}$.

VFR(J,JM) = difference form of $\frac{(\alpha - 1)V\phi}{R}$, where $\phi = 2S_x + S_z$.

PH(J,JM) = interpolation formula to evaluate ϕ at a region boundary where ϕ is discontinuous.

VV(J,JM) = interpolation formula to evaluate V at a region boundary where V is discontinuous.

Local Variables

I = do loop index for region #.

JMN = JMIN for region I
JMX = JMAX for region I } minimum and maximum cell #'s in a region.

J = do loop index for cell #.

JM = J - 1.

JP = J + 1.

D = the last term inside brackets of Eq. 8.

FM = $M_j/(M_j + M_{j+1})$.

MRM = region # for cell J - 1.

MR = region # for cell J.

MRP = region # for cell J + 1.

II = IE(I) = original region # for region I.

Care must be taken that interfaces between materials are treated properly. The differential equation for acceleration is given by

$$\frac{\partial u}{\partial t} = -R^{\alpha-1}\frac{\partial \sigma}{\partial M} - (\alpha - 1)\frac{\phi}{R\rho} \quad . \tag{1}$$

Now, consider an interface between material 1 and material 2 at radius R_0. The difference in the limit of Eq. (1) as R tends to R_0 from region 1 and region 2 is given by

$$-\frac{\partial u_1}{\partial t} + \frac{\partial u_2}{\partial t} = R^{\alpha-1}\left(\frac{\partial \sigma_1}{\partial M_1} - \frac{\partial \sigma_2}{\partial M_2}\right) + (\alpha - 1)\left(\frac{\phi_1}{R\rho_1} - \frac{\phi_2}{R\rho_2}\right) = 0 \quad , \tag{2}$$

where the subscripts denote the region from which the limit is taken. The difference in acceleration is zero provided the two regions are in contact.

For the case $\phi_1 = \phi_2 = 0$, Eq. (2) implies $\partial\sigma_1/\partial M_1 = \partial\sigma_2/\partial M_2$ at R_0. The usual difference equation schemes don't encounter any problems at the interface because $\partial\sigma/\partial M$ is continuous.

For the case $\phi_1 \neq \phi_2$, set $\Delta = (\phi_2/R^{\alpha}\rho_2 - \phi_1/R^{\alpha}\rho_1)(\alpha - 1)$. We then have

$$\frac{\partial \sigma_1}{\partial M_1} - \frac{\partial \sigma_2}{\partial M_2} = \Delta \quad . \tag{3}$$

That is, $\partial\sigma/\partial M$ is not continuous across the interface. Therefore, care must be taken so that the interface will be treated properly by the difference equations.

Let j be the cell number of the cell touching the interface in region 1 and j+1 for region 2. Equation (3) can be written in difference form as

$$\frac{\sigma_j - \sigma_{j+\frac{1}{2}}}{\frac{1}{2}M_j} - \frac{\sigma_{j+\frac{1}{2}} - \sigma_{j+1}}{\frac{1}{2}M_{j+1}} = \Delta \quad , \tag{4}$$

where $\sigma_{j+\frac{1}{2}}$ is unknown. Solving for $\sigma_{j+\frac{1}{2}}$, we have

$$\sigma_{j+\frac{1}{2}} = (M_j + M_{j+1})^{-1}\left(M_{j+1}\sigma_j + M_j\sigma_{j+1} - \left(\frac{\Delta}{2}\right)M_jM_{j+1}\right) \quad . \tag{5}$$

The difference form for $\partial\sigma_1/\partial M_1$ then becomes

$$\frac{\partial\sigma_1}{\partial M_1} = \frac{2}{M_j + M_{j+1}}\left(\sigma_j - \sigma_{j+1} + \frac{\Delta}{2}M_{j+1}\right) \quad . \tag{6}$$

The difference form of the acceleration in region 1 at the boundary is given by

$$\frac{\partial u_1}{\partial t} = -\left[\frac{2R^{\alpha-1}}{M_j + M_{j+1}}\left(\sigma_j - \sigma_{j+1} + \frac{\Delta}{2}M_{j+1}\right) + (\alpha - 1)\frac{\phi_1 V_1}{R}\right] \quad . \tag{7}$$

The velocity equation can then be written in the form

$$u_{j+\frac{1}{2}}^{n+\frac{1}{2}} = u_{j+\frac{1}{2}}^{n-\frac{1}{2}} - \Delta t\left\{(R_{j+\frac{1}{2}})^{\alpha-1}\, 2(\sigma_j - \sigma_{j+1})/(M_j + M_{j+1}) + \frac{(\alpha - 1)}{R_{j+\frac{1}{2}}}\Phi\right\} \quad , \tag{8}$$

where

$$\Phi = \phi_1 V_1\left(\frac{M_j}{M_j + M_{j+1}}\right) + \phi_2 V_2\left(\frac{M_{j+1}}{M_j + M_{j+1}}\right) \quad , \tag{9}$$

with the subscript 1 and 2 denoting the region from which the limit is taken approaching the interface. These limits are taken by extrapolation.

```
      SUBROUTINE SINX                                                    SINX      2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,          PARAM     2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                   PARAM     3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                     PARAM     4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                         PARAM     5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                          MCELL     2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)    MCELL     3
     +,W(MCL)                                                            MCELL     4
      LEVEL 2,R                                                          MCELL     5
      COMMON/DVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM,  MCELL     6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                     MCELL     7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                   MCELL     8
      LEVEL 2,TIME                                                       MCELL     9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO  INIT      2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML),  INIT      3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)             INIT      4
      COMMON/USUPC/C1(ML),S1(ML),C2(ML),S2(ML),SWV(ML),VMN(ML),          US        2
     +GAMMA(ML),ALP(ML)                                                  US        3
      COMMON/MNMX/KMAX(ML2),KMIN(ML2),NMC                                MN        2
      COMMON/VOID/INTX(ML2),JV(ML2),IV(ML2),NNV                          VD        2
      COMMON/ES/IE(ML2),NME                                              ESM       2
      COMMON/UCJC/UCJ,JJ,NMAX,RCJ,DCJ                                    UC        2
      DIMENSION UU(MCL),VO(MCL)                                          SINX     11
      DSDM(J,JM)=2*R(J)**IA*(P(JM)+Q(JM)-P(J)-Q(J))/(XM(J)+XM(JM))       SINX     12
      VFR(J,JM)=IA*(V(J)+V(JM))*(2*(SX(J)+SX(JM))+SZ(J)+SZ(JM))/(4*R(J)) SINX     13
      PH(J,JM)=2*SX(J)+SZ(J)+XM(J)*(2*(SX(J)-SX(JM))-SZ(J)+SZ(JM))/      SINX     14
     +(XM(J)+XM(JM))                                                     SINX     15
      VV(J,JM)=V(J)+XM(J)*(V(J)-V(JM))/(XM(J)+XM(JM))                    SINX     16
      NCLP=NCL+1                                                         SINX     17
      DO 10 J=1,NCLP                                                     SINX     18
      UU(J)=U(J)      Save old u's                                       SINX     19
10    CONTINUE                                                           SINX     20
      DO 20 I=1,NMC                                                      SINX     21
      JMN=JMIN(I)                                                        SINX     22
      JMX=JMAX(I)                                                        SINX     23
      IF(I.NE.1)JMN=JMN+1                                                SINX     24
      DO 21 J=JMN,JMX                                                    SINX     25
      JM=J-1                                                             SINX     26
      U(J)=U(J)-DT*DSDM(J,JM)                                            SINX     27
      IF(INTX(I).GT.2) U(J)=U(J)-DT*VFR(J,JM)                            SINX     28
      R(J)=R(J)+DT*U(J)                                                  SINX     29
21    CONTINUE                                                           SINX     30
      IF(JMAX(I).NE.KMAX(I))GO TO 20                                     SINX     31
      IF(I.EQ.NMC.AND.NMC.NE.NM)GO TO 20                                 SINX     32
      IF(IV(I))31,32,33                                                  SINX     33
31    J=JMX+1                                                            SINX     34
      GO TO 22                                                           SINX     35
32    J=JMX+1                                                            SINX     36
      JP=J+1                                                             SINX     37
      U(J)=U(J)-DT*2*R(J)**IA*(P(JMX)+Q(JMX))/XM(JMX)                    SINX     38
      R(J)=R(J)+DT*U(J)                                                  SINX     39
      U(JP)=U(JP)+DT*2*R(JP)**IA*(P(JP)+Q(JP))/XM(JP)                    SINX     40
      R(JP)=R(JP)+DT*U(JP)                                               SINX     41
      GO TO 20                                                           SINX     42
33    J=JMX+2                                                            SINX     43
22    CONTINUE                                                           SINX     44
      GO TO (1,2,3,4,5),INTX(I)                                          SINX     45
5     U(J)=U(J)-DT*VFR(J,JMX)                                            SINX     46
1     U(J)=U(J)-DT*DSDM(J,JMX)                                           SINX     47
      R(J)=R(J)+DT*U(J)                                                  SINX     48
```

```
      IF(IV(I).EQ.-1)GO TO 20                                          SINX       49
      U(J-1)=U(J)                                                      SINX       50
      R(J-1)=R(J)                                                      SINX       51
      GO TO 20                                                         SINX       52
3     D=IA*(PH(JMX,JMX-1)*VV(JMX,JMX-1)*XM(JMX)/(XM(J)                 SINX       53
     1 +XM(JMX)))/R(J)                                                 SINX       54
      GO TO 6                                                          SINX       55
2     D=IA*PH(J,J+1)*VV(J,J+1)*XM(J)/((XM(J)+XM(JMX))*R(J))            SINX       56
      GO TO 6                                                          SINX       57
4     FM=XM(J)/(XM(J)+XM(JMX))                                         SINX       58
      D=IA*(PH(J,J+1)*VV(J,J+1)*FM+PH(JMX,JMX-1)*VV(JMX,JMX-1)*(1-FM)) SINX       59
     1 /R(J)                                                           SINX       60
6     U(J)=U(J)-DT*(D+DSDM(J,JMX))                                     SINX       61
      R(J)=R(J)+U(J)*DT                                                SINX       62
      IF(IV(I).EQ.-1)GO TO 20                                          SINX       63
      U(J-1)=U(J)                                                      SINX       64
      R(J-1)=R(J)                                                      SINX       65
20    CONTINUE                                                         SINX       66
      CALL BNDR1                                                       SINX       67
      DO 13 I=1,NMC                                                    SINX       68
      JMN=JMIN(I)                                                      SINX       69
      JMX=JMAX(I)                                                      SINX       70
      II=IE(I)                                                         SINX       71
      IF(IV(I).NE.0)GO TO 101                                          SINX       72
      JI=JV(I)                                                         SINX       73
      P(JI)=0.                                                         SINX       74
      Q(JI)=0.                                                         SINX       75
  101 CONTINUE                                                         SINX       76
      DO 12 J=JMN,JMX                                                  SINX       77
      VO(J)=V(J)       Save old V's                                    SINX       78
      V(J)=((R(J)+R(J+1))/2)**IA*(R(J)-R(J+1))/XM(J)                   SINX       79
      JM=J-1                                                           SINX       80
      IF(J.EQ.JMN.AND.IV(I-1).GE.1.AND.I.NE.1)JM=J-2                   SINX       81
      JP=J+1                                                           SINX       82
      IF(J.EQ.KMAX(I).AND.IV(I).GE.1)JP=J+2                            SINX       83
      IF(J.EQ.2.AND.BU.NE.0.)JM=2                                      SINX       84
      IF(JJ.EQ.J+1)JP=J                                                SINX       85
      XI(J)=XI(J)-DT*(((XM(J)*(P(JM)+Q(JM))+XM(JM)*(P(J)+Q(J)))        SINX       86
     1/(XM(J)+XM(JM)))*U(J)*R(J)**IA-((XM(JP)*(P(J)+Q(J))              SINX       87
     2+XM(J)*(P(JP)+Q(JP)))/(XM(J)+XM(JP)))*U(J+1)*R(J+1)**IA)        SINX       88
     3/XM(J)   Δ energy - Δ kinetic energy                             SINX       89
     4+((UU(J+1)+UU(J))**2-(U(J)+U(J+1))**2)/8                         SINX       90
      IF(XMU(II).EQ.0.) GO TO 12                                       SINX       91
      SX(J)=SX(J)+2*XMU(II)*(DT*(U(J)-U(J+1))/(R(J+1)-R(J))+2*(V(J)-   SINX       92
     +VO(J))/(3*(VO(J)+V(J))))                                         SINX       93
      SZ(J)=-SX(J)/2                                                   SINX       94
12    CONTINUE                                                         SINX       95
   13 CONTINUE                                                         SINX       96
      CALL VISC                                                        SINX       97
      DO 60 I=1,NMC                                                    SINX       98
      II=IE(I)                                                         SINX       99
   60 IF(IBRN(II).GT.0)CALL BURN(I)                                    SINX      100
      CALL EOS                                                         SINX      101
      DO 80 I=1,NM                                                     SINX      102
      II=IE(I)                                                         SINX      103
      JMN=JMIN(I)                                                      SINX      104
      JMX=JMAX(I)                                                      SINX      105
      IF(IV(I).EQ.2)CALL RLEOS(I)                                      SINX      106
   80 CONTINUE                                                         SINX      107
      CALL BNDR2                                                       SINX      108
      RETURN                                                           SINX      109
      END                                                              SINX      110
```

SINX

The main hydro cycle using the SIN difference equations. New values of radii, velocities, specific volumes, specific internal energies, and stress deviators are calculated. Subroutines are called to get new pressures, temperatures, and artificial viscosities.

Local Variables (Those variables that are the same as in HYDRO are not repeated here.)

JI = JV(I) = cell # of a void.

NCLP = NCL + 1.

UU = velocity from previous cycle.

VO = volume from previous cycle.

Notes

The difference equation for acceleration is identical with HYDROX. The internal energy equation, however, is based on the total energy equation

$$\frac{\partial E}{\partial t} = - \frac{(\sigma u R^{\alpha-1})}{\partial M} \quad ,$$

which is essentially the rate of PdV work being done on the cell. The rate of change of kinetic energy is then subtracted to get the rate of change of internal energy.

```
      SUBROUTINE EOS                                                    EOS         2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM       2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM       3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM       4
     +,NSM=4,NWPM=3728,NSC=NSM*NWPM+132,ML2=100)                        PARAM       5
      COMMON/CELL/P(MCL),U(MCL),V(MCL),XI(MCL),                         MCELL       2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)   MCELL       3
     +,W(MCL)                                                           MCELL       4
      LEVEL 2,R                                                         MCELL       5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM, MCELL       6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                    MCELL       7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                  MCELL       8
      LEVEL 2,TIME                                                      MCELL       9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO  INIT        2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT        3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)            INIT        4
      COMMON/MNMX/KMAX(ML2),KMIN(ML2),NMC                               MN          2
      COMMON/EOSN/IEOS(ML),ME(ML)                                       EN          2
      COMMON/ES/IE(ML2),NME                                             ESM         2
      COMMON/EOSCOM/SR(ML),ES(ML),A1(ML),A2(ML),A3(ML),EM(ML),IRV(ML)   EOSCOM       2
      COMMON/SESIN/II,IDT,RPT4,XIPT4,IBR,IFL                            EOS        11
      COMMON/SESOUT/PPT4(3),TPT4(3)                                     EOS        12
      IBR=0                                                             EOS        14
      IDT=1                                                             EOS        15
      I=1                                                               EOS        16
   20 CONTINUE                                                          EOS        17
      II=IE(I)    Original region #                                     EOS        18
      IS=IEOS(II)  EOS type                                             EOS        19
      JMN=JMIN(I)                                                       EOS        20
      JMX=JMAX(I)                                                       EOS        21
      GO TO (1,2,3,4),IS                                                EOS        22
    1 CONTINUE                                                          EOS        23
      JS=0                                                              EOS        24
      DO 11 J=JMN,JMX                                                   EOS        25
      CALL HOM(II,J)    HOM EOS                                         EOS        26
      IF(IBRN(II).NE.0)GO TO 11                                         EOS        27
      IF(P(J).LT.-0.005)CALL SPEOS(I,J)  Spall?                         EOS        28
      IF(XMU(II).GT.0.)CALL EPP(II,J)  Elastic - perfectly plastic      EOS        29
   11 CONTINUE                                                          EOS        30
      GO TO 10                                                          EOS        31
    2 CONTINUE                                                          EOS        32
      DO 12 J=JMN,JMX                                                   EOS        33
   12 CALL BLDUP(II,J)  Buildup EOS                                     EOS        34
      GO TO 10                                                          EOS        35
    3 CONTINUE                                                          EOS        36
      JS=0                                                              EOS        37
      DO 13 J=JMN,JMX                                                   EOS        38
      CALL POLY(II,J)  Eight-parameter polynomial EOS                   EOS        39
      IF(P(J).LT.-0.005)CALL SPEOS(I,J)  Spall?                         EOS        40
      IF(XMU(II).GT.0.)CALL EPP(II,J)  Elastic - perfectly plastic      EOS        41
   13 CONTINUE                                                          EOS        42
      GO TO 10                                                          EOS        43
    4 DO 14 J=JMN,JMX                                                   EOS        45
      XIPT4=XI(J)                                                       EOS        46
      RPT4=1./V(J)          ] Input for SESAME                          EOS        47
      IFL=MOD(IFLAG(J),64)  ]                                           EOS        48
      CALL T4EOSA     SESAME EOS                                        EOS        49
      IF(MOD(IFLAG(J),64).EQ.1) GO TO 140                               EOS        50
      IF(IRV(I).EQ.0.AND.IFL.EQ.1) IFLAG(J)=IFLAG(J)+1                  EOS        51
  140 P(J)=PPT4(1)    Output pressure                                   EOS        52
```

```
      T(J)=TPT4(1)    Output temperature                                    EOS        53
      IF(XMU(II).GT.0.)CALL EPP(II,J)   Elastic - perfectly plastic         EOS        54
      IF(P(J).LT.-0.005)CALL SPEOS(I,J)  Spall?                             EOS        55
   14 CONTINUE                                                              EOS        56
   10 CONTINUE                                                              EOS        61
      IF(JS.NE.0)CALL SL(I)   Spall if indicated                            EOS        62
      I=I+1                                                                 EOS        63
      IF(I.LE.NMC) GO TO 20   Spalling changes the # of regions, so a do loop EOS      64
      RETURN                                                 is not used    EOS        65
      END                                                                   EOS        66
```

EOS

Switching routine to call the appropriate equation of state. The spalling and elastic-plastic treatments are also called if turned on.

Local Variables

I = region #.

II = original region #.

IS = EOS #.

JMN,JMX = minimum and maximum active cell #.

```
      SUBROUTINE PTEOS(I,PI,TII,VI,XII)                                 PTEOS      2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM      2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM      3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM      4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                        PARAM      5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                         MCELL      2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)   MCELL      3
     +,W(MCL)                                                           MCELL      4
      LEVEL 2,R                                                         MCELL      5
      COMMON/OVL/NDE,NT,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM, MCELL      6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                    MCELL      7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                  MCELL      8
      LEVEL 2,TIME                                                      MCELL      9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO  INIT       2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT       3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QQ(ML),TMLT(ML),TMC(ML)            INIT       4
      COMMON/EOSN/IEOS(ML),ME(ML)                                       EN         2
      COMMON/ES/IE(ML2),NME                                             ESM        2
      COMMON/SESIN/II,IDT,RPT4,XIPT4,IBR,IFL                            PTEOS      9
      COMMON/SESOUT/PPT4(3),TPT4(3)                                     PTEOS     10
      IDT=1                                                             PTEOS     11
      IBR=1                                                             PTEOS     12
      II=IE(I)                                                          PTEOS     14
      J=JMIN(I)                                                         PTEOS     15
      PT=P(J)      ]                                                    PTEOS     16
      TT=T(J)      |                                                    PTEOS     17
      VT=V(J)      | Set cell quantities in temporary storage           PTEOS     18
      XIT=XI(J)    ]                                                    PTEOS     19
      V(J)=VI      ]                                                    PTEOS     20
      XI(J)=XII    ] Replace by input values                            PTEOS     21
      IS=IEOS(II)                                                       PTEOS     22
      GO TO (1,2,3,4),IS   Call EOS                                     PTEOS     23
    1 CALL HOM(II,J)                                                    PTEOS     24
      GO TO 10                                                          PTEOS     25
    2 CALL BLDUP(II,J)                                                  PTEOS     26
      GO TO 10                                                          PTEOS     27
    3 CALL POLY(II,J)                                                   PTEOS     28
      GO TO 10                                                          PTEOS     29
    4 DO 14 J=JMN,JMX                                                   PTEOS     31
      XIPT4=XI(J)                                                       PTEOS     32
      PPT4=1./V(J)                                                      PTEOS     33
      IFL=MOD(IFLAG(J),64)                                              PTEOS     34
      CALL T4EOS                                                        PTEOS     35
      P(J)=PPT4(1)                                                      PTEOS     36
   14 CONTINUE                                                          PTEOS     37
   10 CONTINUE                                                          PTEOS     42
      PI=P(J)      ]                                                    PTEOS     43
      TII=T(J)     ] Output P,T                                         PTEOS     44
      P(J)=PT                                                           PTEOS     45
      T(J)=TT      ]                                                    PTEOS     46
      V(J)=VT      | Put back original cell quantities                  PTEOS     47
      XI(J)=XIT    ]                                                    PTEOS     48
      RETURN       ]                                                    PTEOS     49
      END                                                               PTEOS     50
```

PTEOS

Controls calls to EOS subroutines with energy and volume as input rather than region # and cell #.

Local Variables

IS = EOS type.

J = cell # used for EOS calls.

PT	temporary storage for	P(J)
TT		T(J)
VT		V(J)
XIT		XI(J).

Notes

EOS calls are made by specifying region # and cell # in this code. In the special treatment of high-velocity void collapse (see RL), it is necessary to call the EOS with arbitrary values of V and I. This is done by saving the cell quantities for a given cell, replacing them with arbitrary values, calling the EOS, returning P,T, and then putting the original cell quantities back in their proper place.

```
      SUBROUTINE HOM(I,J)                                                HOM        2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,          PARAM      2
     +NUMV=10,MOL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                   PARAM      3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                     PARAM      4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                         PARAM      5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                          MCELL      2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)    MCELL      3
     +,W(MCL)                                                            MCELL      4
      LEVEL 2,R                                                          MCELL      5
      COMMON/OVL/NOF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM,  MCELL      6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                     MCELL      7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                   MCELL      8
      LEVEL 2,TIME                                                       MCELL      9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO  INIT       2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT       3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)             INIT       4
      COMMON/MNMX/KMAX(ML2),KMIN(ML2),NMC                                MN         2
      COMMON/EOSN/IEOS(ML),ME(ML)                                        EN         2
      DATA GASW/0.02/                                                    HOM        8
      DATA SOLW/0.999/                                                   HOM        9
C FIXUP FOR FOREST FIRE                                                  HOM       10
      IF(IBRN(I).EQ.0) GO TO 11  All solid                               HOM       11
      IF(W(J).LT.GASW)GO TO 12   Treat as all gas for W < 0.02           HOM       12
      IF(IBRN(I).EQ.2)GO TO 13   Special for CJ burn                     HOM       13
      IF(W(J).GT.SOLW) GO TO 11  Treat as all solid for W > 0.999        HOM       14
      CALL MIX(I,J)   Mixture of gas and solid                           HOM       15
      GO TO 10                                                           HOM       16
11    CONTINUE                                                           HOM       17
      CALL USUP(I,J)   All solid                                         HOM       18
      GO TO 10                                                           HOM       19
12    CALL GAS(I,J)   All gas                                            HOM       20
      GO TO 10                                                           HOM       21
   13 CONTINUE                                                           HOM       22
      IF(W(J).GT.SOLW)GO TO 14                                           HOM       23
      CALL GAS(I,J)                                                      HOM       24
      P(J)=(1.-W(J))*P(J)   No solid EOS for CJ burn                     HOM       25
      GO TO 10                                                           HOM       26
   14 P(J)=PO(I)                                                         HOM       27
10    CONTINUE                                                           HOM       28
      RETURN                                                             HOM       29
      END                                                                HOM       30
```

HOM

Switching routine for deciding which type of EOS is used for a cell for the HOM EOS (e.g., determines whether a material is a solid, gas, or mixture).

Local Variables

GASW = mass fraction below which a material is treated as all gas (W = 0).

SOLW = mass fraction above which a material is treated as all solid (W = 1).

Notes

If a CJ burn is used for an HE, the MIX EOS is not used for partially decomposed HE. Instead, the GAS EOS is used with the pressure weighted by 1-W. For other burn methods (except for sharp shock which never allows partially burned HE), partially decomposed HE (GASW<W<SOLW) is treated in the MIX EOS.

```
      SUBROUTINE USUP(I,J)                                                  USUP      2
C     EQUATION OF STATE FOR A SOLID USING USUP FIT                          USUP      3
C     FOR TWO PHASE FE TYPE EQUATION OF STATE                               USUP      4
C     I.E., C AND S IN THE RELATION US=C+S*UP CHANGE                        USUP      5
C     AT SPECIFIC VOLUME SWV                                                USUP      6
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,             PARAM     2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                      PARAM     3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                        PARAM     4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                            PARAM     5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                             MCELL     2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)       MCELL     3
     +,W(MCL)                                                               MCELL     4
      LEVEL 2,R                                                             MCELL     5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM,     MCELL     6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                        MCELL     7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                      MCELL     8
      LEVEL 2,TIME                                                          MCELL     9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO     INIT      2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML),    INIT      3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)                INIT      4
      COMMON/USUPC/C1(ML),S1(ML),C2(ML),S2(ML),SWV(ML),VMN(ML),             US        2
     +GAMMA(ML),ALP(ML)                                                     US        3
      COMMON/FGHIJC/FS(ML),GS(ML),HS(ML),SI(ML),SJ(ML),CV(ML)               FG        2
      COMMON/BRNS/A(ML),BR(ML),BA(ML),VBO(ML),VBSW(ML)                      BRN       2
      DATA CF/1.39528394E-5/                                                USUP     13
      IF(V(J).LT.VBSW(I)) GO TO 30   Barnes EOS for V < VBSW                USUP     14
      IF(V(J).GT.VO(I))GO TO 40  Grüneisen EOS (with P = 0 reference) for   USUP     15
      IF(V(J).GT.SWV(I))GO TO 11 ]                              tension     USUP     16
      IF(V(J).LT.VMN(I))GO TO 12 |                                          USUP     17
      V(J)=VMN(I)                |   2nd USUP fit used for phase change      USUP     18
12    C=C2(I)                    |                                          USUP     19
      S=S2(I)                    ]                                          USUP     20
      GO TO 20                                                              USUP     21
11    C=C1(I)                                                               USUP     22
      S=S1(I)                                                               USUP     23
20    VOMV=VO(I)-V(J)                                                       USUP     24
      HP=((C/(VO(I)-S*VOMV))**2)*VOMV+PO(I)]  P,I on the Hugoniot           USUP     25
      HE=(HP+PO(I))*VOMV*0.5               ]                                USUP     26
      P(J)=HP+(XI(J)-HE)*GAMMA(I)/V(J)  Shift off the Hugoniot with constant γ USUP  27
C     IF NO HEAT CAPACITY SKIP TEMP CALCULATION                             USUP     28
      IF(CV(I))22,22,21                                                     USUP     29
21    ALNV=ALOG(V(J))                                                       USUP     30
      T(J)=(XI(J)-HE)*23890./CV(I)+EXP(FS(I)+ALNV*(GS(I)+ALNV*(HS(I)        USUP     31
     1+ALNV*(SI(I)+ALNV*SJ(I)))))   Temperature fit                         USUP     32
   22 RETURN                                                                USUP     33
   30 CONTINUE                                                              USUP     34
      CALL BEOST(I,J)  Barnes EOS                                           USUP     35
      RETURN                                                                USUP     36
   40 CONTINUE                                                              USUP     37
      IF(ALP(I))51,51,52                                                    USUP     38
51    P(J)=PO(I)]  Default values for tension if α ≤ 0                      USUP     39
      T(J)=TO(I)]                                                           USUP     40
      RETURN                                                                USUP     41
   52 P(J)=(GAMMA(I)*(XI(J)+(1.-V(J)/VO(I))*CV(I)*CF/ALP(I)))/V(J)          USUP     42
      T(J)=XI(J)*23890./CV(I)+TO(I)  EOS for tension                        USUP     43
      RETURN                                                                USUP     44
      END                                                                   USUP     45
```

USUP

USUP EOS allows for two USUP fits with a phase change. At high density the Barnes EOS is used. In tension, the Grüneisen EOS with the P=0 line as the standard curve is used.

Local Variables

C,S = constants used in USUP fit. $U_S = C + SU_P$ where U_S is the shock velocity and U_P is the particle velocity.

VOMV = $V_0 - V$, where V_0 is the initial specific volume (cm^3/g).

HP = pressure on the Hugoniot for volume V.

HE = energy on the Hugoniot for volume V.

ALNV = $\ell n(V)$

CF = conversion factor in the Grüneisen EOS.

Notes

USUP EOS: For many materials, a plot of U_S versus U_P data is a straight line to a good approximation over the range of interest. The data is then fit to the equation

$$U_S = C + SU_P \quad . \tag{1}$$

This equation combined with the Rankine-Hugoniot equations gives sufficient information to determine the Hugoniot pressure, P_H, and Hugoniot specific internal energy, I_H, on the Hugoniot as a function of the density, ρ, initial density, ρ_0, initial pressure, P_0, and the initial specific internal energy, I_0. The Rankine-Hugoniot equations (also called jump conditions) are given from conservation of mass, momentum, and energy, and from the assumption that the shape of the shock front is constant in time. (For a derivation of these equations see, for example, Courant and Freidrichs, Sec. 54.) The jump conditions are

$$\rho_0 U_S = \rho(U_S - U_P) \quad , \tag{2}$$

$$P_H - P_0 = \rho_0 U_S U_P \quad , \tag{3}$$

$$\left[(I_H - I_0) - \frac{U_P^2}{2}\right]\rho_0 U_S = P_0 U_P \quad . \tag{4}$$

After some algebraic manipulation, the four equations yield the results:

$$P_H = \left(\frac{C}{V_0 - S(V_0 - V)}\right)^2 (V_0 - V) + P_0 \quad , \tag{5}$$

and

$$I_H = \frac{1}{2}(V_0 - V)(P_H + P_0) \quad , \tag{6}$$

where

$$V_0 = \frac{1}{\rho_0} \text{ and } V = \frac{1}{\rho} \quad . \tag{7}$$

Of course, P and I are required off the Hugoniot too. The Grüneisen gamma is defined as $\gamma = V(\partial P/\partial I)_V$. If γ is known, a Taylor expansion around the Hugoniot values for a given specific volume yields (to first order)

$$P = P_H + (I - I_H)\left(\frac{\partial P}{\partial I}\right)_V = P_H + \frac{(I - I_H)\gamma}{V} \quad . \tag{8}$$

For this subroutine, γ is assumed to be constant.

The temperature on the Hugoniot, T_H, is calculated by the method of Walsh and Christian. For the USUP fit, an analytic solution for the Hugoniot temperature can be found, but it involves an exponential integral. So, $\ell n(T_H)$ is fit to a polynomial in $\ell n(V)$, that is,

$$\ell n\ T_H = F + G(\ell n\ V) + H(\ell n\ V)^2 + I(\ell n\ V)^3 + J(\ell n\ V)^4 \quad , \tag{9}$$

with the assumption that $C_V = \left(\frac{\partial I}{\partial T}\right)_V$ is constant, we obtain for temperatures off the Hugoniot

$$T = T_H + \frac{I - I_H}{C_V} \quad . \tag{10}$$

This temperature calculation uses approximately 10% of the CPU time per cell per cycle. So, the temperature should not be calculated unless it will be used (for example, melt criteria, mixture of solid and gas products, etc.).

In tension, the reference pressure, P_r, is zero instead of P_H. At $V = V_0$ the values of T and I are denoted T_1 and I_1, respectively. Using

$$\left(\frac{\partial T}{\partial I}\right)_P = \frac{1}{C_P} \quad , \tag{11}$$

and the assumption that C_P and C_V are indistinguishable and C_V is constant, we have for the reference temperature

$$T_r = T_1 + \frac{I_r - I_1}{C_V} \quad . \tag{12}$$

For $P = 0$,

$$\left(\frac{\partial I}{\partial V}\right)_P = \frac{C_P}{3\alpha V} \quad . \tag{13}$$

With a different assumption about C_V,

$$C_P/3\alpha V = C_V/3\alpha V_0 = \text{constant} \quad , \tag{14}$$

we have

$$I_r = I_1 + \frac{C_V}{3\alpha V_0}(V - V_0) \quad . \tag{15}$$

For this reference energy and $P_r = 0$, the Grüneisen EOS becomes

$$P = \frac{\gamma}{V}\left(I - I_1 - \frac{C_V}{3\alpha V_0}(V - V_0)\right) \quad . \tag{16}$$

Also,

$$T = T_r + \frac{I - I_r}{C_V} \quad . \tag{17}$$

In order to have continuous P and T at I = 0, V = V_0, we find

$$I_1 = \frac{-P_0 V_0}{\gamma} \tag{18}$$

and

$$T_1 = T_0 - \frac{P_0 V_0}{C_V \gamma} \quad . \tag{19}$$

It can be shown that $\left(\frac{\partial P}{\partial V}\right)_S$ will be continuous at V = V_0, P = P_0 for

$$\gamma C_V \doteq 3\alpha C^2 \quad . \tag{20}$$

If this relation is not satisfied, there will be a "bend" in the isentrope.

For further details, see the memo "Consistent EOS Input for HOM" by J. N. Johnson.

```
      SUBROUTINE GAS(I,J)                                                GAS        2
C  EQUATION OF STATE FOR GAS ONLY                                        GAS        3
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,          PARAM      2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                   PARAM      3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                     PARAM      4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                         PARAM      5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                          MCELL      2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)    MCELL      3
     +,W(MCL)                                                            MCELL      4
      LEVEL 2,R                                                          MCELL      5
      COMMON/OVL/NDF,NT,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM,  MCELL      6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),TJK                     MCELL      7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                   MCELL      8
      LEVEL 2,TIME                                                       MCELL      9
      COMMON/GASC/GC(NGC,ML)                                             GC         2
      DIMENSION G(MLGC)                                                  GAS        7
      EQUIVALENCE (GC,G)                                                 GAS        8
      K=(I-1)*NGC                                                        GAS        9
  110 ALNV=ALOG(V(J))   ℓn V                                             GAS       10
      ALNPI=G(K+1)+ALNV*(G(K+2)+ALNV*(G(K+3)+ALNV*(G(K+4)+ALNV*G(K+5))   GAS       11
     1))   ℓn Pi                                                         GAS       12
      ALNII=G(K+6)+ALNPI*(G(K+7)+ALNPI*(G(K+8)+ALNPI*(G(K+9)+ALNPI*G(K   GAS       13
     1+10))))  ℓn Ii'                                                    GAS       14
      ALNTI=G(K+11)+ALNV*(G(K+12)+ALNV*(G(K+13)+ALNV*(G(K+14)+ALNV*G(K   GAS       15
     1+15))))    ℓn Ti                                                   GAS       16
      EI=EXP(ALNII)-G(K+17)   Ii                                         GAS       17
      P(J)=EXP(ALNPI)+(EI-XI(J))/V(J)*(G(K+12)+ALNV*(G(K+13)+G(K+13)+    GAS       18
     1ALNV*(3.*G(K+14)+ALNV*4.*G(K+15))))   P = Pi + (I - Ii)/βV         GAS       19
      T(J)=EXP(ALNTI)+(XI(J)-EI)*23890./G(K+16)  T = Ti + (I - Ii)/Cv     GAS       20
      RETURN                                                             GAS       21
      END                                                                GAS       22
```

GAS

Calculates the EOS for gases using analytic fits to the results of the BKW code. By special choice of constants, a γ-law gas EOS may be calculated.

Local Variables

G = one-dimensional array equivalenced to the two-dimensional array GC.

K = index to locate the data for region I in G.

NGC = parameter = # of gas constants per region.

ALNV = $\ell n\ V_g$.

ALNPI = $\ell n\ P_i$.

ALNII = $\ell n\ I_i'$.

ALNTI = $\ell n\ T_i$.

EI = $I_i' - Z = I_i$.

Notes

The BKW equation of state for the gaseous products is

$$PV_g/RT = 1 + xe^{\beta x} \quad , \tag{1}$$

where V_g is the molar volume of the gaseous products and

$$x = \frac{\kappa k}{V_g(T + \theta)^{\alpha}} \quad , \tag{2}$$

where

$$k = \sum_g x_i k_i \quad , \tag{3}$$

with $x_i = n_i/n_g$ being the mole fraction of gaseous compound i, k_i is a constant covolume for that compound, and κ,α,β are constants fit to reproduce detonation data. Also, there may be solid products such as graphite. The mole fractions will vary with volume and temperature. The equilibrium

composition is calculated by minimization of the Gibbs free energy. Space does not permit a complete discussion of the EOS calculation in the BKW code. The interested reader is referred to Appendix E of Numerical Modeling of Detonations by C. L. Mader. Analytic fits are made in the BKW code to reference values of pressure (P_i), specific internal energy (I_i) and temperature (T_i) on the adiabat going through the CJ point. The fits used are given by

$$\ell n\ P_i = G_1 + G_2(\ell n\ V) + G_3(\ell n\ V)^2 + G_4(\ell n\ V)^3 + G_5(\ell n\ V)^4 \quad , \tag{4}$$

$$\ell n\ I_i' = G_6 + G_7(\ell n\ P_i) + G_8(\ell n\ P_i)^2 + G_9(\ell n\ P_i)^3 + G_{10}(\ell n\ P_i)^4 \quad , \tag{5}$$

$$\ell n\ T_i = G_{11} + G_{12}(\ell n\ V) + G_{13}(\ell n\ V)^2 + G_{14}(\ell n\ V)^3 + G_{15}(\ell n\ V)^4 \quad , \tag{6}$$

$$I_i = \exp\ (\ell n\ I_i') - Z \quad , \tag{7}$$

where Z is a constant such that I_i has the same energy zero as the solid EOS. Also, Z can be used to keep I_i' positive when making a fit.

The Grüneisen EOS is

$$P = P_i + \frac{\gamma}{V}\ (I - I_i) \quad , \tag{8}$$

where

$$\gamma = V\left(\frac{\partial P}{\partial I}\right)_V \quad . \tag{9}$$

We can use the thermodynamic relation

$$\left(\frac{\partial P}{\partial I}\right)_V = \left(\frac{\partial P}{\partial S}\right)_V \left(\frac{\partial S}{\partial I}\right)_V = -\frac{1}{T}\left(\frac{\partial T}{\partial V}\right)_S \tag{10}$$

to write γ in terms of the function β defined by

$$-\frac{1}{\beta} = \left(\frac{\partial\ \ell n\ T}{\partial\ \ell n\ V}\right)_S = \frac{V}{T}\left(\frac{\partial T}{\partial V}\right)_S \quad , \tag{11}$$

giving

$$\gamma = \frac{1}{\beta} \quad . \tag{12}$$

We can readily evaluate β since $\ell n\ T_i$ on the adiabat is fit as a function of $\ell n\ V$. The result is

$$-\frac{1}{\beta} = G_{12} + 2G_{13}\ell n\ V + 3G_{14}(\ell n\ V)^2 + 4G_{15}(\ell n\ V)^3 \quad . \tag{13}$$

The pressure is then given by

$$P = P_i + \frac{I - I_i}{\beta V} \quad . \tag{14}$$

With the assumption of constant C_V, the temperature is

$$T = T_i + \frac{(I - I_i)}{C_V} \quad . \tag{15}$$

```
      SUBROUTINE SSBGAS(I,J)                                                SSBGAS     2
C     SHARP SHOCK BURN                                                      SSBGAS     3
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,             PARAM      2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                      PARAM      3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                        PARAM      4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                            PARAM      5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                             MCELL      2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)       MCELL      3
     +,W(MCL)                                                               MCELL      4
      LEVEL 2,R                                                             MCELL      5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM,     MCELL      6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                        MCELL      7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                      MCELL      8
      LEVEL 2,TIME                                                          MCELL      9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO     INIT       2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML),    INIT       3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)                INIT       4
      COMMON/GASC/GC(NGC,ML)                                                GC         2
      COMMON/ES/IE(ML2),NME                                                 ESM        2
      COMMON/BUX/BUA,BUB,BUMAX,BUDV(ML)                                     BUP        2
     +,BUR,BUD                                                              BUP        3
      COMMON/EOSN/IEOS(ML),ME(ML)                                           EN         2
      DIMENSION G(MLGC)                                                     SSBGAS    11
      EQUIVALENCE (GC,G)                                                    SSBGAS    12
      II=IE(I)                                                              SSBGAS    13
      IF(IEOS(I).EQ.2)GO TO 2                                               SSBGAS    14
      K=(I-1)*NGC                                                           SSBGAS    15
  110 ALNV=ALOG(V(J))   ℓn V                                                SSBGAS    16
      ALNPI=G(K+1)+ALNV*(G(K+2)+ALNV*(G(K+3)+ALNV*(G(K+4)                   SSBGAS    17
     ++ALNV*G(K+5))))   ℓn P_j                                              SSBGAS    18
      ALNII=G(K+6)+ALNPI*(G(K+7)+ALNPI*(G(K+8)+ALNPI*(G(K+9)                SSBGAS    19
     ++ALNPI*G(K+10))))   ℓn I'_j                                           SSBGAS    20
      EI=EXP(ALNII)-G(K+17)   I_j                                           SSBGAS    21
  111 SIP=EXP(ALNPI)   P_j                                                  SSBGAS    22
      GAV=(G(K+12)+ALNV*(G(K+13)*2+ALNV*(3*G(K+14)+ALNV*4*G(K+15))))        SSBGAS    23
     +/V(J)   -1/βV                                                         SSBGAS    24
      P(J)=(SIP+FI*GAV)/(1+0.5*(VO(I)-V(J))*GAV)  P on Hugoniot              SSBGAS    25
      XI(J)=0.5*P(J)*(VO(I)-V(J))  I on Hugoniot                            SSBGAS    26
      RETURN                                                                SSBGAS    27
    2 CONTINUE  Buildup EOS                                                 SSBGAS    28
      WPCJ=BUDV(I)*ROW(I)/(T(J)+1.)   P_CJ                                  SSBGAS    29
      WVCJ=T(J)*VO(I)/(T(J)+1.)    V_CJ                                     SSBGAS    30
      WBI=T(J)*(T(J)-2.32)/(T(J)-.66)  1/β                                  SSBGAS    31
      WK=-0.5*BUDV(I)/(T(J)*T(J)-1.)  I_∞                                   SSBGAS    32
      WPI=WPCJ*(WVCJ/V(J))**T(J)   P_1                                      SSBGAS    33
      P(J)=(WPI-(WK+WPI*V(J)/(T(J)-1))/(WBI*V(J)))/   P on Hugoniot          SSBGAS    34
     +(1-(VO(II)-V(J))/(2*WBI*V(J)))                                        SSBGAS    35
      XI(J)=P(J)*(VO(II)-V(J))/2  I on Hugoniot                             SSBGAS    36
      RETURN                                                                SSBGAS    37
      END                                                                   SSBGAS    38
```

SSBGAS

Calculates the pressure and specific internal energy for a cell that has just been burned using the sharp-shock burn method. The pressure and specific internal energy are calculated on the Hugoniot for the HE products at the given volume.

Local Variables

G = one-dimensional array equivalenced to the two-dimensional array GC

K = index to locate the data for region I in G

NGC = parameter = # of gas constants per region

ALNV = $\ell n\ V_g$

ALNPI = $\ell n\ P_i$

ALNII = $\ell n\ I_i'$

EI = $I_i' - Z = I_i$

$S_{IP} = P_i$

GAV = $-\frac{1}{\beta V}$

Notes

In the sharp shock burn (see subroutine SSB for more details) a cell is compressed to CJ volume without going through the hydrodynamic equations. So, it is necessary to find the Hugoniot pressure, P_H, and specific internal energy, I_H, from the jump conditions and the equation of state. The jump condition for specific internal energy is

$$I_H = \frac{1}{2}(V_0 - V)(P_H + P_0) \quad . \tag{1}$$

For detonations, P_0 is negligible. The equation of state for the HE products is

$$P = \frac{1}{\beta V}(I - I_i) + P_i \quad , \tag{2}$$

where I_i and P_i are functions of volume only (see subroutine GAS). By using I_H from Eq. (1) for I in Eq. (2) and solving for $P = P_H$, we have

$$P_H = \frac{P_i - I_i/\beta V}{1 - (V_0 - V)/2\beta V} \cdot \tag{3}$$

Then using the value of P_H, I_H follows from Eq. (1).

```
      SUBROUTINE MIX(I,J)                                                    MIX        2
C  EQUATION OF STATE FOR MIXTURE OF SOLID AND GAS                            MIX        3
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,              PARAM      2
     +NUMV=10,MOL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                       PARAM      3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                         PARAM      4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                             PARAM      5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                              MCELL      2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)        MCELL      3
     +,W(MCL)                                                                MCELL      4
      LEVEL 2,R                                                              MCELL      5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UTI,UFI,NADD,NM,      MCELL      6
     +IALPH,NDELT,LAGFL(8),NDUMP,IDMP,NM1,TD(ML),IJK                         MCELL      7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                       MCELL      8
      LEVEL 2,TIME                                                           MCELL      9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO      INIT       2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML),     INIT       3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)                 INIT       4
      COMMON/USUPC/C1(ML),S1(ML),C2(ML),S2(ML),SWV(ML),VMN(ML),              US         2
     +GAMMA(ML),ALP(ML)                                                      US         3
      COMMON/GASC/GC(NGC,ML)                                                 GC         2
      COMMON/FGHIJC/FS(ML),GS(ML),HS(ML),SI(ML),SJ(ML),CV(ML)                FG         2
      DIMENSION G(MLGC)                                                      MIX       10
      EQUIVALENCE (GC,G)                                                     MIX       11
      DIMENSION VIT(10)                                                      MIX       12
      DATA VIT(3)/1.E-5/  Tolerance for solution: pressure equilibrium within MIX       13
      DATA VIT(10)/0./                                  10^-5 Mbar           MIX       14
      DATA VGSS/0.65/                                                        MIX       15
      XLM=1.01*VO(I)*(S1(I)-1.)/S1(I)  1.01 times V at which Hugoniot pressure MIX     16
      K=(I-1)*NGC                                       is infinite          MIX       17
  210 OMW=1.-W(J)                                                            MIX       18
      OMWR=1./OMW                                                            MIX       19
      IF (V(J).LT.VO(I)) GO TO 230  Iterate on Vs for V < V0; Vg for V > V0  MIX       20
      WR=1./W(J)                                                             MIX       21
      VIT(1)=(V(J)-W(J)*VO(I)*VGSS)*OMWR  1st guess for Vg: assume Vs =      MIX       22
      VIT(2)=0.998  Ratio to get next point             VGSS*VO(I)           MIX       23
C     IBR=1 FOR ITERATION ON VG                                              MIX       24
      IBR=1                                                                  MIX       25
  215 CALL LFB (X,F,VIT)  One step of iteration                              MIX       26
      IF (VIT(10)) 900,260,220  Error, solution, continue iteration          MIX       27
  220 IF (X.LE.0.) GO TO 225  For fixup when X = Vg becomes unphysical       MIX       28
      VG=X                  ] New values for Vg,Vs                           MIX       29
      VS=(V(J)-OMW*VG)*WR   ]                                                MIX       30
      IF (VS.LE.0.) GO TO 225  For fixup                                     MIX       31
      GO TO 250                                                              MIX       32
C     SET VS=VG=VOLUME WHEN GET IN TROUBLE                                   MIX       33
  225 VS=V(J)           ]                                                    MIX       34
      VG=V(J)           ] Attempted fixup when iteration gives unphysical values MIX     35
      X=V(J)            ]                                                    MIX       36
      GO TO 250                                                              MIX       37
  230 VIT(1)=V(J)  1st guess for Vs                                          MIX       38
      VIT(2)=.999  Ratio to get 2nd point                                    MIX       39
C     IBR=2 FOR ITERATION ON VS                                              MIX       40
      IBR=2                                                                  MIX       41
  235 CONTINUE                                                               MIX       42
      IF(F.LT.10.0.AND.X.GT.XLM)GO TO 236 ]                                  MIX       43
      X=(X+VIT(4))/2                      ] Don't allow Vs to get near or    MIX       44
      GO TO 240                           ]  below the singularity in pressure MIX     45
  236 CALL LFB(X,F,VIT)  One step of iteration                               MIX       46
      IF (VIT(10)) 900,260,240  Error, solution, continue iteration          MIX       47
  240 IF (X.LE.0.) GO TO 225  For fixup                                      MIX       48
```

```
      VS=X                          ]  New values for Vs,Vg                    MIX        49
      VG=(V(J)-W(J)*VS)*OMWR        ]                                          MIX        50
      IF (VG.LE.0.) GO TO 225                                                  MIX        51
C     CALCULATE TEMPERATURE/PRESSURE DIFFERENCE FOR MIXTURE ITERATION          MIX        52
  250 VOMV=VO(I)-VS                                                            MIX        53
      HP=((C1(I)/(VO(I)-S1(I)*VOMV))**2)*VOMV   PH                             MIX        54
      HE = (HP-P0(I))*VOMV*0.5   IH                                            MIX        55
      ALNV=ALOG(VS)   ℓn Vs                                                    MIX        56
      HT=EXP(FS(I)+ALNV*(GS(I)+ALNV*(HS(I)+ALNV*(SI(I)+ALNV*SJ(I))))) TH       MIX        57
      ALNV=ALOG(VG)   ℓn Vg                                                    MIX        58
      ALNPI=G(K+1)+ALNV*(G(K+2)+ALNV*(G(K+3)+ALNV*(G(K+4)+ALNV*G(K+5))))       MIX        59
      IF(ALNPI.LT.G(K+19))ALNPI=G(K+19)  ℓn Pi, limit of validity on ℓn Ii fit MIX        60
      EI=EXP(G(K+6)+ALNPI*(G(K+7)+ALNPI*(G(K+8)+ALNPI*(G(K+9)+ALNPI*G(         MIX        61
     1K+10)))))-                                                               MIX        62
     1G(K+17)  Ii                                                              MIX        63
      PI=EXP(ALNPI)  Pi                                                        MIX        64
      TI=EXP(G(K+11)+ALNV*(G(K+12)+ALNV*(G(K+13)+ALNV*(G(K+14)+ALNV*G(         MIX        65
     1K+15))))  Ti                                                             MIX        66
      IF(ALNV.GT.G(K+18))ALNV=G(K+18) Limit of validity of 1/β fit             MIX        67
      BETER=-(G(K+12)+ALNV*(G(K+13)+G(K+13)+ALNV*(3.*G(K+14)+4.*ALNV*G         MIX        68
     1(K+15))))  1/β                                                           MIX        69
      TEMP=-G(K+16)*BETER/VG  -C'V V/βVg                                       MIX        70
      TEMP1=GAMMA(I)*CV(I)/VS  γCV/Vs                                          MIX        71
      F=-(HT*TEMP1+TI*TEMP)*4.18585182E-5  -[(THγsCV/Vs) - (TiC'V/βVg)]        MIX        72
      TEMP=TEMP+TEMP1  Equilibrium temperature                                 MIX        73
      VSTO=(CV(I)-G(K+16))*W(J)+G(K+16)  WCV + (1 - W)C'V                      MIX        74
      F=((OMW*G(K+16)*TI+W(J)*CV(I)*HT)*4.18585182E-5+(EI-HE)*W(J)-EI+         MIX        75
     1XI(J))*TEMP/VSTO+F-PI+HP  Pressure difference = fi(X)                    MIX        76
      GO TO (215,235),IBR                                                      MIX        77
C     HAVE FOUND A SOLUTION FOR THE MIXTURE                                    MIX        78
C     GET THE TEMPERATURE AND PRESSURE                                         MIX        79
  260 VARST=((((TI-HT)*G(K+16)*4.18585182E-5+XI(J)*OMWR-EI)*CV(I)+HE*G         MIX        80
     1(K+16))*OMW/VSTO)-HE  I - IH                                             MIX        81
      P(J)=HP+VARST*GAMMA(I)/VS  ]  Output P,T                                 MIX        82
      T(J)=HT+VARST*23890./CV(I) ]                                             MIX        83
      RETURN                                                                   MIX        84
C     ERROR IN HOM ITERATION       SET IND TO -1                               MIX        85
  900 IND=-1                                                                   MIX        86
      PRINT 901,TIME,I,J,X,F,VIT,VS,VG,IBR                                     MIX        87
  901 FORMAT(1X,10H HOM ERROR,E12.5,2I5,4E12.5/10F12.5,I5)                     MIX        88
      RETURN                                                                   MIX        89
      END                                                                      MIX        90
```

MIX (I,J)

Calculates pressure and temperature for a mixture of solid and gas where temperature and pressure are assumed to be in equilibrium. The equations of state for the solid and gas are described more fully in USUP and GAS, respectively.

Local Variables

VIT = array of dimension 10 used by LFB (q.v.) for the iterative solution.

VGSS = relative specific volume assumed for the solid for the first guess when iteration is on V_g.

K = index to locate the data for region I in G.

OMW = 1 - W.

OMWR = $(1 - W)^{-1}$.

WR = 1/W.

IBR = 1 for iteration on V_g; 2 for iteration on V_s.

X = current value of the iteration variable: updated by LFB.

F = current value of the iteration function: calculated in MIX.

VG = V_g.

VS = V_s.

HP = P_H.

HE = I_H.

HT = T_H.

ALNV = $\ell n\ V_g$ or $\ell n\ V_s$.

ALNPI = $\ell n\ P_i$.

EI = I_i.

PI = P_i.

TI = T_i.

BETER = $1/\beta$.

TEMP = $-C_V'/\beta V_g$.

TEMP1 = $\gamma_s C_V / V_s$.

VSTO = $WC_V + (1 - W)C_V'$.

VARST = $I - I_H$ in equilibrium.

IND = error index.

Notes

The solid equations used are

$$P_H = \frac{C^2(V_0 - V_s)}{[V_0 - S(V_0 - V_s)]^2} \quad , \tag{1}$$

$$\ln T_H = F_s + G_s \ln V_s + H_s(\ln V_s)^2 + I_s(\ln V_s)^3 + J_s(\ln V_s)^4 \quad , \tag{2}$$

$$I_H = \frac{1}{2} P_H(V_0 - V_s) \quad , \tag{3}$$

$$P_s = \frac{\gamma_s}{V_s} (I_s - I_H) + P_H \quad , \tag{4}$$

$$T_s = T_H + \frac{I_s - I_H}{C_V} \quad , \tag{5}$$

where the s subscript denotes quantities associated with the solid.

The gas equations used are

$$\ln P_i = A + B \ln V_g + C(\ln V_g)^2 + D(\ln V_g)^3 + E(\ln V_g)^4 \quad , \tag{6}$$

$$\ln I_i' = K + L(\ln P_i) + M(\ln P_i)^2 + N(\ln P_i)^3 + O(\ln P_i)^4 \quad , \tag{7}$$

$$I_i = I_i' - Z \quad , \tag{8}$$

$$\ln T_i = Q + R \ln V_g + S(\ln V_g)^2 + T(\ln V_g)^3 + U(\ln V_g)^4 \quad , \tag{9}$$

$$-\frac{1}{\beta} = R + 2S(\ln V_g) + 3T(\ln V_s)^2 + 4U(\ln V_g)^3 \quad , \tag{10}$$

$$P_g = \frac{1}{\beta V_g}(I_g - I_i) + P_i \quad , \tag{11}$$

$$T_g = T_i + \frac{I_g - I_i}{C_V'} \quad , \tag{12}$$

where the g subscript denotes quantities associated with the gas.

The equilibrium conditions are

$$P = P_g = P_s \quad , \tag{13}$$

$$T = T_g = T_s \quad , \tag{14}$$

where P and T are the pressure and temperature of the mixture.

Two more relations are easily derived from the definition of mass fraction:

$$V = WV_s + (1 - W)V_g \quad , \tag{15}$$

$$I = WI_s + (1 - W)I_g \quad , \tag{16}$$

where V and I are the specific volume and specific internal energy of the mixture.

Multiplying Eq. (5) by WC_V and Eq. (12) by $(1 - W)C_V'$ we have, after adding and substituting Eq. (14) and Eq. (16),

$$T = \frac{[I - (WI_H + (1 - W)I_i) + WC_V T_H + (1 - W)C_V' T_i]}{WC_V + (1 - W)C_V'} \quad , \tag{17}$$

which is an expression for the equilibrium temperature as a function of V_s and V_g (which are related by Eq. (15)).

Combining Eqs. (4), (11), and (13), we have

$$\frac{\gamma_s}{V_s}(I_s - I_H) + P_H = \frac{1}{\beta V_g}(I_g - I_i) + P_i \quad . \tag{18}$$

Combining Eqs. (5), (12), and (14), we have

$$I_s - I_H = C_V(T - T_H) \tag{19}$$

and

$$I_g - I_i = C_V'(T - T_i) \quad . \tag{20}$$

So the equation for pressure equilibrium (with equilibrium temperature T from Eq. (17)) may be written in the form

$$f(V_s,V_g) = P_H - P_i + \left(\frac{\gamma_s C_V}{V_s} - \frac{C_V'}{\beta V_g}\right)T - \left(\frac{\gamma_s C_V T_H}{V_s} - \frac{C_V' T_i}{\beta V_g}\right) = 0 \quad . \tag{21}$$

Using Eq. (16), this equation can be reduced to either of two functions of one variable:

$$f_1(V_g) = f\left(\frac{V - (1 - W)V_g}{W}\ ,\ V_g\right) = 0 \tag{22}$$

or

$$f_2(V_s) = f\left(V_s\ ,\ \frac{V - WV_s}{1 - W}\right) = 0 \quad . \tag{23}$$

Since the pressure for the mixture is always positive, V_s will not get much larger than V_0 (thermal expansion at low pressure). So, for $V > V_0$, $f_2(V_s)$ will be very sensitive to the value of V_s. Therefore, Eq. (22) is solved for $V > V_0$ and Eq. (23) is solved for $V < V_0$. The solution is found by an iterative technique, basically the secant method, described in LFB. The method requires two starting points to be stored in VIT(1) and VIT(2) where x_1 = VIT(1) and x_2 = VIT(1) * VIT(2). For iteration on V_s, VIT(1) is chosen to be V. For iteration on V_g, VIT(1) is chosen such that V_s is V_0 * VGSS. Sometimes the iteration will begin to diverge and give unphysical values such as negative V_s or V_g. The standard fixup is to set $V_g = V_s = V$ which does not always work. Currently, if the iteration fails to converge, the old values of P,T are used and an error message is printed. Usually,

for cases where the iteration fails to converge for several cycles for the same cell, the problem will become unstable and an error (usually due to a negative volume) will occur, stopping the problem.

Two of the fits used in the GAS equation of state are not always accurate for large V_g. The constants G(K + 18) and G(K + 19) provide limits on the valid regions of the fits. Further detail can be found in GASLM.

The function f is the difference in pressure of the gas and solid when they are in thermal equilibrium. So, the value of VIT(3) (which is the tolerance allowed in a solution) is the absolute limit of the accuracy in megabars. The standard limit is 10^{-5} Mbar.

```
      SUBROUTINE LFB(XP,FP,TX)                                          LFB        2
C      TX(1)      INITIAL GUESS                                         LFB        3
C      TX(2)      RATIO TO GET SECOND POINT                             LFB        4
C      TX(3)      ZERO DEFINITION                                       LFB        5
C      TX(10)     COUNT OF NUMBER OF ITERATIONS                         LFB        6
C                 SET TO ZERO ON SOLUTION                               LFB        7
C                 SET TO NEGATIVE OF COUNT ON ERROR                     LFB        8
C      FP         =FUNCTION(XP)                                         LFB        9
C      WHEN A SOLUTION IS FOUND, XP IS THE ROOT                         LFB       10
C                                                                       LFB       11
C      ERROR EXITS OCCUR FOR                                            LFB       12
C            1. TOO MANY ITERATIONS, .GT.CNTMAX                         LFB       13
C            2. TWO SUCESSIVE XP S OR FP S ARE EQUAL                    LFB       14
      DIMENSION TX(10)                                                  LFB       15
      DATA CNTMAX /100./                                                LFB       16
      IF (TX(10).LE.0.) GO TO 1                                         LFB       17
      TX(10)=TX(10)+1.                                                  LFB       18
      IF (TX(10)-3.) 2,3,4                                              LFB       19
C  ENTRY FIRST TIME THROUGH                                             LFB       20
    1 TX(10)=1.                                                         LFB       21
      IF (TX(1).EQ.0.) TX(1) = 1.                                       LFB       22
      XP=TX(1)   x0                                                     LFB       23
C  GO GET F(XP)   f(x0)                                                 LFB       24
      RETURN                                                            LFB       25
C  ENTRY SECOND TIME THROUGH                                            LFB       26
    2 TX(9)=FP   f(x0)                                                  LFB       27
      TX(8)=XP   x0                                                     LFB       28
      TX(5)=FP                                                          LFB       29
      IF (ABS(FP).LT.TX(3)) GO TO 18   Solution?                        LFB       30
      XP=TX(1)*TX(2)   x1                                               LFB       31
C  GO GET F(XP)                                                         LFB       32
      RETURN                                                            LFB       33
C  ENTRY THIRD TIME THROUGH                                             LFB       34
    3 TX(5)=FP   f(x1)                                                  LFB       35
      TX(6)=XP   x1                                                     LFB       36
      TX(4)=XP   x1                                                     LFB       37
      TX(7)=FP   f(x1)                                                  LFB       38
      IF (ABS(FP).LT.TX(3)) GO TO 18   Solution?                        LFB       39
      XP=TX(5)-TX(7)*(TX(6)-TX(8))/(TX(7)-TX(9))   x2                   LFB       40
C  GO GET F(XP)   f(x2)                                                 LFB       41
      RETURN                                                            LFB       42
C  ENTRY FOR FOURTH AND SUCEEDING TIMES THROUGH                         LFB       43
    4 IF (TX(10).GT.CNTMAX) GO TO 99                                    LFB       44
      TX(4)=XP   xj                                                     LFB       45
      TX(5)=FP   f(xj)                                                  LFB       46
      T=TX(4)-TX(5)   xj - xj-1                                         LFB       47
      IF (T.EQ.0.) GO TO 99                                             LFB       48
      IF (ABS(FP).LT.TX(3)) GO TO 18   Solution                         LFB       49
      R=TX(5)-TX(7)   f(xj) - f(xj-1)                                   LFB       50
      IF (R.EQ.0.) GO TO 99                                             LFB       51
      XP=TX(4)-TX(5)*(T/R)   xj+1 by Eq. (1)                            LFB       52
      IF (TX(5)*TX(7).LT.0.) GO TO 11 ]                                 LFB       53
      IF (TX(5)*TX(9).GE.0.) GO TO 11 ]  See notes                      LFB       54
      IF (XP.GT.TX(4)) GO TO 6        ]                                 LFB       55
      IF (XP.GT.TX(8)) GO TO 10       ]                                 LFB       56
    8 XP=TX(4)-TX(5)*(TX(4)-TX(8))/(TX(5)-TX(9))   xj+1 by Eq. (2)       LFB       57
   10 TX(7)=TX(5) ]                                                     LFB       58
      TX(6)=TX(4) ]  See notes                                          LFB       59
C  GO GET F(XP)   ]                                                    LFB       60
      RETURN                                                            LFB       61
```

```
     6 IF (XP.GT.TX(8)) GO TO 8                                    LFB        62
       GO TO 10                                                    LFB        63
    11 TX(9)=TX(7)]                                                LFB        64
       TX(8)=TX(6)]    See notes                                   LFB        65
       GO TO 10                                                    LFB        66
C   HAVE FOUND A SOLUTION                                          LFB        67
    18 TX(10)=0.   Index for solution                              LFB        68
       TX(1)=XP                                                    LFB        69
       TX(4)=XP                                                    LFB        70
       RETURN                                                      LFB        71
C   AN ERROR HAS OCCURED                                           LFB        72
C   SET COUNT NEGATIVE AND EXIT                                    LFB        73
    99 TX(10)=-TX(10)   Index for error                            LFB        74
       RETURN                                                      LFB        75
       END                                                         LFB        76
```

LFB(XP,FP,TX)

A two-point iteration scheme to find the zero of a function of one variable. The iteration is a slightly modified form of the secant method. This method is faster than Newton-Raphson iteration for the case where the time required to evaluate the derivative is longer than 0.44 of the time required to evaluate the function.

Local Variables

XP = estimated value of the root from the previous iterative step.

FP = value of the function at XP.

TX = array containing current and previous values of XP and FP.

Also, TX(1) = initial guess for XP; TX(2) = ratio to get second XP; TX(3) = error limit, TX(10) = count of iterations.

T = TX(4) - TX(6).

R = TX(5) - TX(7).

Notes

The secant method for finding a root of f(x) = 0 is given by

$$x_{i+1} = x_i - \left(\frac{x_i - x_{i-1}}{y_i - y_{i-1}}\right) y_i \quad , \tag{1}$$

where $y_i = f(x_i)$. Two points, x_0 and x_1, are required to begin the iteration.

The secant method is used in LFB with the restriction that if $y_i y_{i-1} > 0$ and $y_i y_{i-2} < 0$ with x_{i+1} not between x_i and x_{i-2}, then

$$x_{i+1} = x_i - \left(\frac{x_i - x_{i-2}}{y_i - y_{i-2}}\right) y_i \quad . \tag{2}$$

This modification treats the case where a root is known to be between x_i and x_{i-2} from the fact that $y_i y_{i-2} < 0$. If $y_i y_{i-1} > 0$, then there is the

possibility that x_{i+1} from Eq. (1) is not between x_i and x_{i-2}. (If that is the case, then Eq. (2) is used for x_{i+1}, which will then give x_{i+2} between x_i and x_{i-2}.) This modification helps avoid divergence of the solution in some cases. When Eq. (2) is used, x_{i-1} is replaced by x_{i-2} and y_{i-1} is replaced by y_{i-2}. The relation of x_i and y_i to TX in the code is as follows

$TX(4) = x_i$

$TX(5) = y_i$

$TX(6) = x_{i-1}$

$TX(7) = y_{i-1}$

$TX(8) = x_{i-2}$

$TX(9) = y_{i-2}$

```
      SUBROUTINE BEOST(I,J)                                              BEQST      2
C     BARNES SOLID EQUATION OF STATE                                     BEQST      3
C     ROUTINE SETS VOLUMES GREATER THAN VO TO VO AND ENERGIES LESS       BEQST      4
C     THAN ZERO DEGREE ENERGY TO ZERO DEGREE ENERGY                      BEQST      5
      REAL  N,NU,IC                                                      BEQST      6
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,          PARAM      2
     +NUMV=10,MVL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                   PARAM      3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                     PARAM      4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                         PARAM      5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                          MCELL      2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)    MCELL      3
     +,W(MCL)                                                            MCELL      4
      LEVEL 2,R                                                          MCELL      5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UTI,UFI,NADD,NM,  MCELL      6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                     MCELL      7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                   MCELL      8
      LEVEL 2,TIME                                                       MCELL      9
      COMMON/BRNS/A(ML),BR(ML),BA(ML),VBO(ML),VBSW(ML)                   BRN        2
      DIMENSION E1BR(ML),EXBR(ML)                                        BEQST     10
C     VOLUME CAN NOT BE GREATER THAN VO                                  BEQST     11
      DATA E1BR,EXBR/ML*0.,ML*0./                                        BEQST     12
      IF(E1BR(I).NE.0.)GO TO 10                                          BEQST     13
      E1BR(I)=E1(BR(I))  ]                                               BEQST     14
      EXBR(I)=EXP(BR(I))]  Constant for a given material                 BEQST     15
   10 CONTINUE                                                           BEQST     16
      VV=V(J)                                                            BEQST     17
      IF(VV.GT.VBO(I)) VV=VBO(I)                                         BEQST     18
      N=VBO(I)/VV    η                                                   BEQST     19
      CRN = N**(1./3.)   η^1/3                                           BEQST     20
      NU = 1. - 1./CRN   ν                                               BEQST     21
      EBRN=EXP(BR(I)*NU)  exp(b_r ν)                                     BEQST     22
      EBAN=EXP(BA(I)*NU)  exp(b_a ν)                                     BEQST     23
      PC=A(I)*(EBRN*CRN**5-EBAN*CRN*CRN)  P_C                            BEQST     24
      GM=-1./3.+1./18.*((EBRN*(8.*BR(I)*CRN**4   γ                       BEQST     25
     ++18.*CRN**5+BR(I)*BR(I)*N)+EBAN*                                   BEQST     26
     +(-2.*BA(I)*CRN-BA(I)*BA(I)))/(EBRN*(CRN**5                         BEQST     27
     ++1./3.*BR(I)*CRN**4)-EBAN*1./3.*CRN*BA(I)))                        BEQST     28
      BON=BR(I)/CRN  b_r η^-1/3                                          BEQST     29
      IC=3./2.*A(I)*VBO(I)*(EBRN*(CRN**2-BR(I)   I_C                     BEQST     30
     +*CRN)+BR(I)-1.+(2./BA(I))*(1.-EBAN)                                BEQST     31
     +-BR(I)*BR(I)*EXBR(I)*(E1BR(I)-E1(BON)))                            BEQST     32
C     ENERGY CAN NOT BE LESS THAN ZERO DEGREE ENERGY                     BEQST     33
      IF(XI(J).LT.IC)XI(J)=IC                                            BEQST     34
      P(J)=PC+GM*(XI(J)-IC)/VV  Pressure output                          BEQST     35
      PZ=PC                                                              BEQST     36
      RETURN                                                             BEQST     37
      END                                                                BEQST     38
```

BEQST(I,J)

The Barnes EOS is used for the high-pressure region where the USUP fit becomes unphysical.

Local Variables

VV = AMIN (V(J),VBO(I)).

N = $\eta = \frac{V_0}{V}$, where V_0 = VBO(I), V = V(J), and N is declared real.

CRN = $\eta^{1/3}$.

NU = $\nu = 1 - \eta^{-1/3}$. NU is declared real.

EBRN = $e^{b_r\nu}$.

EBAN = $e^{b_a\nu}$.

PC = $P_c = A\eta^{2/3}(\eta e^{b_r\nu} - e^{b_a\nu})$ = pressure on the zero-degree isotherm.

GM = γ calculated by the Dugdale-MacDonald formula using P_c.

BON = $b_r\eta^{-1/3}$.

IC = I_c = specific internal energy of the zero-degree isotherm. IC is declared real.

Notes

The Morse potential has been modified by Barnes to give the proper (i.e., $P \propto \rho^{5/3}$ for free-electron gas) form at very high pressures. The pressure on the zero-degree isotherm, P_c, is given by

$$P_c = a\eta^{2/3}\left(\eta e^{b_r\nu} - e^{b_a\nu}\right) , \qquad (1)$$

where $\eta = V_0/V$, $\nu = 1 - \eta^{-1/3}$, and a, b_r, and b_a are constants. The constants a and b_r are usually chosen such that the repulsive term matches the Thomas-Fermi-Dirac (TFD) pressure at $\eta = 1$ and $\eta = 10$, respectively. The TFD pressure is typically fit within 2% over the range $1 < \eta < 15$ by this

repulsive term. Given a and b_r, then b_a is chosen to match the experimental isothermal bulk modulus, B_0, using

$$B_0 = \left(\frac{dP_c}{d\eta}\right)_{\eta=1} = \frac{1}{3}\, a(3 + b_r - b_a) \quad . \tag{2}$$

The specific internal energy on the zero-degree isotherm, I_c, is given by

$$I_c = -\int_{V_0}^{V} P_c \, dV \quad . \tag{3}$$

Changing variables to $\eta = V_0/V$ gives

$$I_c = V_0 \int_1^{\eta} \frac{P_c(\eta)}{\eta^2}\, d\eta = aV_0 \int_1^{\eta} \left(\eta^{-1/3} e^{b_r \nu} - \eta^{-4/3} e^{b_a \nu}\right) d\eta \quad . \tag{4}$$

Further change of variables to $x = \eta^{-1/3} = 1 - \nu$ gives

$$\begin{aligned} I_c &= -3aV_0 \int_1^{\eta^{-1/3}} \frac{x e^{b_r(1-x)} - x^{+4} e^{b_a(1-x)}}{x^4}\, dx \\ &= +\frac{3}{2} a V_0 \left[-1 + b_r + e^{b_r \nu}\left(\eta^{2/3} - b_r \eta^{1/3}\right) + \frac{2}{b_a}\left(1 - e^{b_a \nu}\right)\right. \\ &\quad \left. -b_r^2 \left(\left[-E_i(-b_r)\right] - \left[-E_i(-b_r \eta^{-1/3})\right]\right)\right] \quad , \end{aligned} \tag{5}$$

where $E_i(x) = \int_{-\infty}^{x} \frac{e^t}{t}\, dt$ is the exponential integral.

The Grüneisen γ is computed using the Dugdale-MacDonald formula:

$$\gamma = -\frac{1}{3} - \frac{V}{2} \frac{\partial^2 (PV^{2/3})/\partial V^2}{\partial (PV^{2/3}) \partial V} \quad , \tag{6}$$

or in terms of η,

$$\gamma = -\frac{1}{3} + \frac{\eta^2 \frac{\partial}{\partial \eta}(PV^{2/3}) + \frac{\eta^3}{2}\frac{\partial^2}{\partial \eta^2}(PV^{2/3})}{\eta^2 \frac{\partial (PV^{2/3})}{\partial \eta}} \quad , \tag{7}$$

where

$$PV^{2/3} = AV_0^{2/3}(\eta e^{b_r \nu} - e^{b_a \nu}) \quad . \tag{8}$$

After evaluating the derivatives and multiplying numerator and denominator by $\eta^{-1/3}$, we have

$$\gamma = -\frac{1}{3} + \frac{1}{18} \frac{e^{b_r \nu}\left(18\eta^{5/3} + 8\, b_r \eta^{4/3} + b_r^2 \eta\right) + e^{b_a \nu}\left(-2b_a \eta^{1/3} - b_a^2\right)}{e^{b_r \nu}\left(\eta^{5/3} + \frac{1}{3} b_r \eta^{4/3}\right) + e^{b_a \nu}\left(-\frac{b_a}{3}\eta^{1/3}\right)} \quad . \tag{9}$$

The pressure is then evaluated using the Grüneisen EOS with P_c and I_c as reference pressure and specific internal energy, respectively,

$$P = P_c + \frac{\gamma \eta}{V_0}(I - I_c) \quad . \tag{10}$$

Care must be taken in choosing the volume, VBSW, below which the Barnes EOS is used instead of the USUP EOS. The Barnes γ depends on volume and the USUP γ is constant. So, for a given volume the two γ's are generally not equal. That means there is only one value of I which gives a continuous pressure at VBSW. Therefore, a value of VBSW chosen to give a continuous pressure on the Hugoniot will not give a continuous pressure along a typical adiabat. So, VBSW may need to be different for different problems. The error due to a wrong choice of VBSW will be enhanced as VBSW decreases. This is due primarily to the increased values of I with smaller volume.

The usual choice of VBSW is to match pressures at the Hugoniot. Using the Hugoniot energy equation

$$E_H = \frac{1}{2}(V_0 - V)P_H = \frac{1}{2}V_0((\eta - 1)/\eta)P_H \tag{11}$$

and the Grüneisen EOS, we can solve for the Hugoniot pressure

$$P_H = \frac{P_c - \gamma(\eta/V_0)E_c}{1 - \gamma(\eta - 1)/2} \tag{12}$$

and compare with USUP Hugoniot to find the proper choice for VBSW.

```
      SUBROUTINE BLDUP(I,J)                                                 BLDUP      2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,             PARAM      2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                      PARAM      3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                        PARAM      4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                            PARAM      5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                             MCELL      2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)       MCELL      3
     +,W(MCL)                                                               MCELL      4
      LEVEL 2,R                                                             MCELL      5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM,     MCELL      6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                        MCELL      7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                      MCELL      8
      LEVEL 2,TIME                                                          MCELL      9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO     INIT       2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML),    INIT       3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)                INIT       4
      COMMON/EOSM/IEOS(ML),ME(ML)                                           EN         2
      COMMON/BUX/BUA,BUB,BUMAX,BUDV(ML)                                     BUP        2
     +,BUR,BUD                                                              BUP        3
      DATA WMAX/0.99/                                                       BLDUP      8
      DATA TL/0./,IL/0/                                                     BLDUP      9
      IF(W(J).GE.WMAX)GO TO 11  Set P = 0 for W > 0.99                      BLDUP     10
      IF(T(J).EQ.TL.AND.I.EQ.IL)GO TO 20  Don't recalculate constants unless BLDUP     11
      TL=T(J)                                                    necessary  BLDUP     12
      IL=I                                                                  BLDUP     13
      WPCJ=BUDV(I)*ROW(I)/(T(J)+1.)  PCJ                                    BLDUP     14
      WVCJ=T(J)*VO(I)/(T(J)+1.)    VCJ                                      BLDUP     15
      WBI=T(J)*(T(J)-2.32)/(T(J)-.66)  1/β                                  BLDUP     16
      WK=-0.5*BUDV(I)/(T(J)*T(J)-1.)  Iβ                                    BLDUP     17
   20 WPI=WPCJ*(WVCJ/V(J))**T(J)   Reference pressure                        BLDUP     18
      PG=WBI*((XI(J)-WK)/V(J)-WPI/(T(J)-1.))+WPI  Pressure for W = 0         BLDUP     19
      P(J)=PG*(1-W(J))  Scaled pressure                                     BLDUP     20
      GO TO 10                                                              BLDUP     21
   11 CONTINUE                                                              BLDUP     22
      P(J)=0.                                                               BLDUP     23
   10 CONTINUE                                                              BLDUP     24
      RETURN                                                                BLDUP     25
      END                                                                   BLDUP     26
```

BLDUP

Calculates the equation of state to be used with the buildup burn model. The EOS is that of a γ-law gas but the γ is not necessarily the same for all cells in a given material.

Local Variables

TL = the value of T(J) = γ for cell J from the last call to BLDUP.

IL = the value of I = original region # from the last call to BLDUP.

WPCJ = P_{CJ} for this cell.

WVCJ = V_{CJ} for this cell.

WBI = $1/\beta$ for this cell.

WK = I_{∞} for this cell.

WPI = the reference pressure, P_r, which is on the isentrope going through the CJ point.

PG = the actual pressure, P_g, which assumes W = 0.

Notes

A number of explosives have been shown to have an effective CJ pressure that varies with distance of run. An effective way of modeling this experimentally observed phenomena is to use a γ-law EOS for the gas products where γ is a function of the distance of run. (See Mader's book for more details.) To a very good approximation, γ has been found to fit the data with the functional form

$$\gamma = A + \frac{B}{X} \quad , \tag{1}$$

where X is the distance of run. The detonation velocity, D, is essentially constant and is assumed to be constant. For short distances of run, γ is not allowed to exceed a maximum value γ_{max} because the functional form for γ becomes inappropriate for small values of X. The buildup model is designed to describe conditions in which the HE is underdriven but promptly detonates. For a sufficiently small input shock, the buildup to detonation requires a non-negligible distance of run and should be calculated with the Forest Fire burn model (see FOREST). The constants for PBX-9404 are A = 2.68, B = 1.39, D = 0.88, and γ_{max} = 3.7.

From the jump conditions and the definition of γ (see, for example, Fickett and Davis for details), the CJ pressure and volume can be expressed as

$$P_{CJ} = \frac{\rho_0 D^2}{\gamma + 1} \tag{2}$$

and

$$V_{CJ} = \frac{\gamma V_0}{\gamma + 1} \quad , \tag{3}$$

where D is the detonation velocity and γ is evaluated at the CJ point.

For buildup EOS we use a γ-law gas as the reference curve with the constant-β EOS off the isentrope. For a given cell, γ is a constant calculated from Eq. (1). With the condition that the reference curve goes through the CJ point, we have for the reference pressure

$$P_i = P_{CJ} V_{CJ}^{\gamma} V^{-\gamma} \quad . \tag{4}$$

The corresponding reference energy is then

$$I_i = \frac{P_i V}{\gamma - 1} + K \quad , \tag{5}$$

where K is a constant appropriate for the zero of energy used. In our case, the energy is defined as zero for the solid explosive. For this zero of energy, the specific internal energy at the CJ point is

$$I_{CJ} = \frac{P_{CJ}(V_0 - V_{CJ})}{2} \quad . \tag{6}$$

Substitution of Eq. (6) in Eq. (5) gives

$$K = - \frac{-P_{CJ}V_{CJ}}{\gamma - 1} + \frac{P_{CJ}}{2} (V_0 - V_{CJ}) = - \frac{D^2}{2(\gamma^2 - 1)} \quad . \tag{7}$$

The constant-β EOS (β is the inverse of the Grüneisen Γ) is given by

$$P = P_i + \frac{1}{\beta V} (I - I_i) \quad . \tag{8}$$

One can determine β at the CJ point from experiment using the following relations (see Fickett and Davis, p. 30):

$$\alpha\beta\gamma = 1 + \alpha \tag{9}$$

and

$$\frac{\partial \ \ell n \ D}{\partial \ \ell n \rho_0} = \frac{\gamma - 1 - \alpha}{2 + \alpha} \quad , \tag{10}$$

to give

$$\beta = \frac{\gamma - \frac{\partial \ \ell n \ D}{\partial \ \ell n \ \rho_0}}{\gamma\left(\gamma - \frac{5}{3} - \frac{\partial \ \ell n \ D}{\partial \ \ell n \ \rho_0}\right)} \quad . \tag{11}$$

For PBX-9404, $\partial \ \ell n \ D / \partial \ \ell n \ \rho_0$ is about 0.66.

Either CJ burn or sharp-shock burn may be used with the buildup model using the CJ volume from Eq. (3) that can vary from cell to cell as γ varies through Eq. (1).

```
      SUBROUTINE SPEOS(I,J)                                              SPEOS     2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,          PARAM     2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                   PARAM     3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                     PARAM     4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                         PARAM     5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                          MCELL     2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)    MCELL     3
     +,W(MCL)                                                            MCELL     4
      LEVEL 2,R                                                          MCELL     5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM,  MCELL     6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                     MCELL     7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                   MCELL     8
      LEVEL 2,TIME                                                       MCELL     9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO  INIT      2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT      3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)             INIT      4
      COMMON/USUPC/C1(ML),S1(ML),C2(ML),S2(ML),SWV(ML),VMN(ML),          US        2
     +GAMMA(ML),ALP(ML)                                                  US        3
      COMMON/SPC/SP(ML),USP(ML)                                          SPLC      2
     +,XISP(ML)                                                          SPLC      3
      COMMON/FGHIJC/FS(ML),GS(ML),HS(ML),SI(ML),SJ(ML),CV(ML)            FG        2
      COMMON/EOSN/IEOS(ML),ME(ML)                                        EN        2
      COMMON/ES/IE(ML2),NME                                              ESM       2
      II=IE(I)                                                           SPEOS    11
      IF(SP(II).LT.0.0001)RETURN   Don't spall for SP < 10-4             SPEOS    12
      JMP=JMAX(I)+1                                                      SPEOS    13
      DPDX=P(J)/(R(J)-R(JMP))  Calculate pressure gradient               SPEOS    14
      IF(J.LE.(JMIN(I)+1)) RETURN ] New regions must have at least 2 cells SPEOS  15
      IF(J.GE.(JMP-2)) RETURN     ]                                      SPEOS    16
      TM=SP(II)*SQRT(-DPDX)                                              SPEOS    17
      SPLP=-TM   Gradient spall pressure                                 SPEOS    18
      IF(TM.GT.USP(II))SPLP=-USP(II)   Ultimate spall pressure           SPEOS    19
      IF(P(J).GT.SPLP)RETURN  Spall?                                     SPEOS    20
      JS=J                                                               SPEOS    21
      RETURN                                                             SPEOS    22
      END                                                                SPEOS    23
```

SPEOS

Determines whether a cell should spall by using the gradient spall model. As a special case, a constant spall pressure may be specified.

Local Variables

II = IE(I) = original region #.

JMP = JMAX(I)+1 = index for the inside radius of the region I.

DPDX = $\frac{dP}{dx}$ assuming pressure is linear and the inside surface is a P = 0.

TM = negative of the gradient spall term.

SPLP = spall pressure.

Notes

An empirical model* that has been found to fit experimental data for spalling is the gradient spall model. The spall pressure is of the form

$$P_s = -A\sqrt{\frac{dP}{dx}} \quad , \tag{1}$$

where $\frac{dP}{dx}$ is the pressure gradient and A is a constant for a given material which is denoted SP(II) in the code for original region II. A locally evaluated numerical value of $\frac{dP}{dx}$ requires a very smooth solution for P vs x in order to be accurate. To avoid possible problems, $\frac{dP}{dx}$ has been approximated by the form

$$\frac{dP}{dx} \cong \frac{\Delta P}{\Delta x} = \frac{P}{x - x_0} \quad , \tag{2}$$

where P is evaluated at x and x_0 is the inside surface of the region in question. The assumptions in this approximation are that the inside surface

*B. R. Breed, Charles L. Mader, Douglas Venable, J. Appl. Phys. 38, 3271 (1967).

of the region is a free surface with $P_0 = 0$, that the pressure is a linear function of distance between x and x_0, and that the direction of motion is toward the inside.

An additional assumption is made that there is an ultimate spall pressure (-USP(II) in the code) at which the material spalls regardless of the stress gradient. So if P_s from Eq. (1) is less than -USP(II), then the spall pressure is set at -USP(II). If a cell meets the criteria for spalling, the flag JS is set to the cell #. The actual spalling is done elsewhere in the code. Since the code requires at least 2 cells in a region, spalling that would create a one-cell region is not allowed.

```
      SUBROUTINE POLY(I,J)                                                  POLY        2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,             PARAM       2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                      PARAM       3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                        PARAM       4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                            PARAM       5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                             MCELL       2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)       MCELL       3
     +,W(MCL)                                                               MCELL       4
      LEVEL 2,R                                                             MCELL       5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM,     MCELL       6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                        MCELL       7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                      MCELL       8
      LEVEL 2,TIME                                                          MCELL       9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO     INIT        2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML),    INIT        3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)                INIT        4
      COMMON/POLYC/CF(NCF,ML),PS(ML)                                        PLC         2
    1 CONTINUE                                                              POLY        7
      VV=VO(I)/V(J)-1.   η                                                  POLY        8
      A=VV*(CF(1,I)+CF(2,I)*ABS(VV))  A                                     POLY        9
      B=CF(3,I)+VV*(CF(4,I)+VV*CF(5,I))  B                                  POLY       10
      C=CF(6,I)+CF(7,I)*VV   C                                              POLY       11
      XIJ=XI(J)*ROW(I)   ε                                                  POLY       12
      P(J)=(A+XIJ*(B+C*XIJ))/(XIJ+CF(8,I))  Pressure output                 POLY       13
   10 CONTINUE                                                              POLY       14
      RETURN                                                                POLY       15
      END                                                                   POLY       16
```

POLY(I,J)

An eight-parameter fit to the equation of state that is basically a polynomial in two variables divided by a linear function in one of the variables. The two variables are related to specific volume and specific internal energy.

Local Variables

VV = $\eta = \frac{V_0 - V}{V}$ (not the same η as in CUSUP).

A = A in the notes (a function of η only).

B = B in the notes (a function of η only).

C = C in the notes (a function of η only).

XIJ = $\rho_0 I$ = initial density * specific internal energy = ε in the notes.

Notes

The coefficients CF(J,I) will be denoted C_J in the notes. The eight-parameter fit for the pressure is given by

$$P = \frac{A + B\varepsilon + C\varepsilon^2}{\varepsilon + C_8} \quad , \tag{1}$$

where

$$A = \eta C_1 + \eta|\eta| C_2 \quad , \tag{2}$$

$$B = C_3 + \eta C_4 + \eta^2 C_5 \quad , \tag{3}$$

$$C = C_6 + \eta C_7 \quad , \tag{4}$$

with

$$\eta = \frac{V_0 - V}{V} \tag{5}$$

and

$$\varepsilon = \rho_0 I \quad . \tag{6}$$

It can be shown that, like the USUP EOS, this EOS has a maximum possible compression on the Hugoniot. However, unlike the USUP EOS, adiabats are well

described at higher compressions. For most (if not all) materials the C_i's are all positive. A positive C_8 means the pressure is finite for finite η and ε. (The Hugoniot pressure goes to infinity at maximum compression because ε does.)

```
      SUBROUTINE VISC                                                   VISC      2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM     2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM     3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM     4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                        PARAM     5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                         MCELL     2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)   MCELL     3
     +,W(MCL)                                                           MCELL     4
      LEVEL 2,R                                                         MCELL     5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM, MCELL     6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                    MCELL     7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                  MCELL     8
      LEVEL 2,TIME                                                      MCELL     9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO  INIT      2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT      3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)            INIT      4
      COMMON/MNMX/KMAX(ML2),KMIN(ML2),NMC                               MN        2
      COMMON/XCOM/R1,R2,DR1,DR2,WO,NCI,DR,ZI                            XC        2
      COMMON/FS/IF(ML2),NME                                             FSM       2
      DO 10 I=1,NMC                                                     VISC      9
      II=IE(I)                                                          VISC     10
      JMN=JMIN(I)                                                       VISC     11
      JMX=JMAX(I)                                                       VISC     12
      DO 10 J=JMN,JMX                                                   VISC     13
      DU=U(J+1)-U(J)  ΔU                                                VISC     14
      IF(ABS(P(J)).LT.QQ(II))GO TO 11                                   VISC     15
      IF(DU.LT.0.0.AND.NV(I).NE.0)GO TO 11                              VISC     16
      IF(NV(I)-1)1,2,3                                                  VISC     17
1     Q(J)=4*XV(I)*DU/(3*V(J)*XM(J))   "Real" (negative Q allowed)      VISC     18
      GO TO 10                                                          VISC     19
2     Q(J)=ABS(XV(I)*(0.5*(U(J)+U(J+1))-UO(I))*DU/V(J))                 VISC     20
      GO TO 10                                                          VISC     21
3     Q(J)=ABS(XV(I)*DU/V(J))  Landshoff                                VISC     22
      GO TO 10                                                          VISC     23
11    Q(J)=0.                                                           VISC     24
10    CONTINUE                                                          VISC     25
      RETURN                                                            VISC     26
      END                                                               VISC     27
```

VISC

Computes the viscosity for all cells using either "real," PIC, or Landshoff-type viscosity.

Local Variables

DU = U(J) - U(J-1) = the change in velocity across a cell.

I = region #.

J = cell #.

JMN,JMX = minimum and maximum active cell #'s in a region.

Notes

For a sufficiently small time step, the difference equations coupled with an equation of state will lead to cell quantities that follow an adiabat, i.e., the entropy will not change. However, in a shock, entropy is not conserved. Without some dissipative mechanism it is impossible to satisfy the energy and momentum jump conditions at a shock front at the same time. That is, the proper pressure jump on the adiabat gives the wrong energy jump and vice versa. (However, for small amplitude shocks the adiabat and the Hugoniot are almost the same since it can be shown that the difference between the two is of third order in the specific volume change, e.g., see Courant and Friedrichs, p. 142.) This and other things lead to oscillations in the cell quantities after the shock front passes.

For most problems, the real viscosity is too small by several orders of magnitude to supply the needed entropy change across the shock front. Two "artificial viscosity" treatments are included in the code. Both are proportional to the velocity change, ΔU, across a cell. The PIC type is also proportional to the change in cell velocity from initial conditions. This effectively scales the viscosity with shock strength so that the shock is smeared over about the same number of cells independent of strength.

```
      SUBROUTINE BURN(I)                                                BURN      2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM     2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM     3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM     4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                        PARAM     5
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO INIT      2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT     3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)            INIT      4
      COMMON/ES/IE(ML2),NME                                             ESM       2
      II=IE(I)                                                          BURN      6
      GO TO (1,2,3,4,5,6,7),IBRN(II)   Index for type of burn           BURN      7
    1 CALL ARH(I)   Arrhenius                                           BURN      8
      GO TO 10                                                          BURN      9
    2 CALL CJ(I)   CJ                                                   BURN     10
      GO TO 10                                                          BURN     11
    3 CALL SSB(I)   Sharp shock                                         BURN     12
      GO TO 10                                                          BURN     13
    4 CALL FOREST(I)   Forest Fire (pressure)                           BURN     14
      GO TO 10                                                          BURN     15
    5 CALL FFT(I)   Forest Fire (temperature)                           BURN     16
      GO TO 10                                                          BURN     17
    6 CALL FFI(I)   Forest Fire (energy)                                BURN     18
      GO TO 10                                                          BURN     19
    7 CALL GLTW(I)   Gamma-law Taylor wave                              BURN     20
 10   CONTINUE                                                          BURN     21
      RETURN                                                            BURN     22
      END                                                               BURN     23
```

BURN(I)

Switching routine to determine type of burn to be used.

Notes

IBRN	Type of Burn
1	Arrhenius
2	CJ
3	Sharp shock
4	Forest Fire
5	Forest Fire rate as a function of temperature
6	Forest Fire rate as a function of internal energy
7	Gamma-law Taylor wave

Any other type of burn may be added by extending the computed go to statement last and adding the subroutine call and the subroutine.

```
      SUBROUTINE ARH(I)                                                 ARH        2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM      2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM      3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM      4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                        PARAM      5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                         MCELL      2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)   MCELL      3
     +,W(MCL)                                                           MCELL      4
      LEVEL 2,R                                                         MCELL      5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM, MCELL      6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                    MCELL      7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                  MCELL      8
      LEVEL 2,TIME                                                      MCELL      9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO  INIT       2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT       3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)            INIT       4
      COMMON/BRND/Z(ML),E(ML),VCJ(ML),DWDT(NDW,ML),PCJ(ML),PM(ML),ND(ML) BRD      2
     +,MSFF                                                             BRD        3
      COMMON/ES/IE(ML2),NME                                             ESM        2
      II=IE(I)                                                          ARH        8
      JMN=JMIN(I)                                                       ARH        9
      JMX=JMAX(I)                                                       ARH       10
      IF(E(II).LT.0.0001) GO TO 11] Don't calculate if constants say don't burn  ARH  11
      IF(Z(II).LT.0.0001) GO TO 11]                                     ARH       12
      DO 10 J=JMN,JMX                                                   ARH       13
      IF(W(J).EQ.0.)GO TO 10  No more to burn                           ARH       14
      IF(T(J).LT.0.0001) GO TO 10  Avoid underflow                      ARH       15
      W(J)=W(J)*(1.-DT*Z(II)*EXP(-E(II)/(1.9865*T(J)))) W^-1 dW/dt = Ze^-E/RT  ARH  16
      IF(W(J).LT.0.6)W(J)=0.    Burn the rest of it                     ARH       17
   10 CONTINUE                                                          ARH       18
   11 CONTINUE                                                          ARH       19
      RETURN                                                            ARH       20
      END                                                               ARH       21
```

ARH(I)

Calculates the decomposition due to an Arrhenius rate law for region I.

Local Variables

II = IE(I) = original region #.

JMN = minimum cell #.

JMX = maximum cell #.

J = do loop index = cell #.

Notes

The Arrhenius rate for burn is given by

$$\frac{1}{W}\frac{dW}{dt} = Ze^{-E/RT} \quad , \tag{1}$$

where W is the mass fraction of undecomposed explosive, Z is a frequency factor (μs^{-1}), E is the activation energy in cal/mole, R is the gas constant (1.9865 cal/mole-K), and T is the temperature (K). This corresponds to a thermally activated process where the barrier height is EK/R and the frequency of attempts to cross the barrier is Z.

```
      SUBROUTINE CJ(I)                                                    CJ          2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,           PARAM       2
     +NUMV=10,MOL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                    PARAM       3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                      PARAM       4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                          PARAM       5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                           MCELL       2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)     MCELL       3
     +,W(MCL)                                                             MCELL       4
      LEVEL 2,R                                                           MCELL       5
      COMMON/OVL/NOF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM,   MCELL       6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),TJK                      MCELL       7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                    MCELL       8
      LEVEL 2,TIME                                                        MCELL       9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO   INIT        2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML),  INIT        3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)              INIT        4
      COMMON/BRND/Z(ML),E(ML),VCJ(ML),DWDT(NDW,ML),PCJ(ML),PM(ML),ND(ML)  BRD         2
     +,MSFF                                                               BRD         3
      COMMON/MNMX/KMAX(ML2),KMIN(ML2),NMC                                 MN          2
      COMMON/EOSN/IEOS(ML),ME(ML)                                         EN          2
      COMMON/ES/TE(ML2),NME                                               ESM         2
      II=IE(I)                                                            CJ         10
      JMN=JMIN(I)                                                         CJ         11
      JMX=JMAX(I)                                                         CJ         12
      DO 10 J=JMN,JMX                                                     CJ         13
      WO=W(J)                                                             CJ         14
      IF(IEOS(II).EQ.2) VCJ(II)=T(J)*VO(II)/(T(J)+1)  Buildup VCJ         CJ         15
      W(J)=1.-(VO(II)-V(J))/(VO(II)-VCJ(II))   CJ burn                    CJ         16
      IF(W(J).LT.0.02)W(J)=0.                                             CJ         17
      IF(WO.GT.W(J))GO TO 10   Don't unburn                               CJ         18
      W(J)=WO                                                             CJ         19
      IF(WO.LT.0.9)W(J)=0.                                                CJ         20
10    CONTINUE                                                            CJ         21
      RETURN                                                              CJ         22
      END                                                                 CJ         23
```

CJ(I)

Calculates the decomposition of a detonating HE using the CJ burn model.

Local Variables

II = IE(I) = original region #.

JMN = minimum cell #.

JMX = maximum cell #.

J = do loop index = cell #.

WO = old value of W(J).

Notes

The CJ burn model assumes the burn fraction, W, varies linearly with the specific volume, V, between V_0 and V_{CJ}; that is,

$$W = 1 - \frac{V_0 - V}{V_0 - V_{CJ}} = \frac{V - V_{CJ}}{V_0 - V_{CJ}} \quad . \tag{1}$$

For the buildup EOS (see BLDUP), V_{CJ} is a function of position and is given by

$$V_{CJ} = \frac{\gamma V_0}{\gamma + 1} \quad , \tag{2}$$

where γ depends on position and is stored in the temperature variable.

Several constraints are made on the value of W. If $W < 0.02$ the rest is burned. If $W_{old} < W_{new}$ (i.e., the cell expands) then the old W is still used to prevent "unburning." If this occurs for $W < 0.9$ then the cell is completely burned.

The burn is normally initiated by a piston with the CJ particle velocity. After the detonation is well started (3rd cell in has burned), the piston velocity is switched to the escape velocity of the products.

The CJ burn is appropriate for a case where the HE promptly detonates. Otherwise, the Forest Fire model (see FOREST) will be appropriate.

```
      SUBROUTINE SSB(I)                                                 SSB       2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM     2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM     3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM     4
     +,NSM=4,NWPM=3729,NSD=NSM*NWPM+132,ML2=100)                        PARAM     5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                         MCELL     2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)   MCELL     3
     +,W(MCL)                                                           MCELL     4
      LEVEL 2,R                                                         MCELL     5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM, MCELL     6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                    MCELL     7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                  MCELL     8
      LEVEL 2,TIME                                                      MCELL     9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO  INIT      2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT      3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)            INIT      4
      COMMON/BRND/Z(ML),E(ML),VCJ(ML),DWDT(NDW,ML),PCJ(ML),PM(ML),ND(ML) BRD       2
     +,MSFF                                                             BRD       3
      COMMON/UCJC/UCJ,JJ,NMAX,RCJ,DCJ                                   UC        2
      COMMON/MNMX/KMAX(ML2),KMIN(ML2),NMC                               MN        2
      COMMON/ES/IE(ML2),NME                                             ESM       2
      COMMON/BUX/BUA,BUB,BUMAX,BUDV(ML)                                 BUP       2
     +,BUR,BUD                                                          BUP       3
      COMMON/EOSN/IEOS(ML),ME(ML)                                       EN        2
      DATA ISSB,JJ/1,1/                                                 SSB      12
      II=IE(I)                                                          SSB      13
      IF(JJ.GT.KMAX(I))GO TO 50  New region                             SSB      14
      IF(JJ.LT.KMIN(I))JJ=KMIN(I)                                       SSB      15
      IF(ISSB-4)30,35,35  4 cycles per cell                             SSB      16
30    ISSB=ISSB+1                                                       SSB      17
      P(JJ)=0.                                                          SSB      18
      Q(JJ)=0.                                                          SSB      19
      RETURN                                                            SSB      20
35    ISSB=1                                                            SSB      21
      W(JJ)=0.  Burn the cell                                           SSB      22
      Q(JJ)=0.                                                          SSB      23
      CALL SSBGAS(II,JJ)  Get CJ P,T                                    SSB      24
      IF(IA.EQ.0.AND.IEOS(II).EQ.2)UCJ=-DCJ/(T(JJ+1)+1)  Build up U_CJ  SSB      25
      IF(IA.EQ.0)GO TO 42                                               SSB      26
      DCJ=VO(II)*SQRT(P(JJ)/(VO(II)-V(JJ)))  ] Converging geometry      SSB      27
      UCJ=-SQRT(P(JJ)*(VO(II)-V(JJ)))        ]                          SSB      28
42    DT=((R(JJ+1)-R(JJ+2))/DCJ*0.25)  4 cycles for detonation to cross the cell SSB 29
      JJ=JJ+1  Next cell                                                SSB      30
      NMAX=JJ                                                           SSB      31
      IF(JJ.LE.KMAX(I))U(JJ)=UCJ  Particle velocity for next cell       SSB      32
      RCJ=R(JJ)  Radius                                                 SSB      33
      CALL JMNMX(NMAX)  Activate the next cell                          SSB      34
      IF(NMC.EQ.T)RETURN                                                SSB      35
      IF(II.NE.IE(I))RETURN                                             SSB      36
50    DT=DTO(II+1)  Next region                                         SSB      37
      IBRN(II)=1                                                        SSB      38
      II=IE(I+1)                                                        SSB      39
      IF(IBRN(II).NE.3)GO TO 51                                         SSB      40
      IF(IEOS(II).EQ.2)GO TO 52                                         SSB      41
      UCJ=-E(II)                  ]                                     SSB      42
      DCJ=VCJ(II)                 |                                     SSB      43
      GO TO 53                    | Initial U_CJ, D_CJ for the next region SSB    44
52    DCJ=SQRT(BUDV(II))          |                                     SSB      45
      JMN=JMIN(I+1)               |                                     SSB      46
      UCJ=-DCJ/(T(JMN)+1)         ]                                     SSB      47
```

```
53 CONTINUE                                                        SSB        48
   JJ=KMIN(I+1)-1                                                  SSB        49
   U(JJ+1)=UCJ                                                     SSB        50
   ISSB=0                                                          SSB        51
   GO TO 42                                                        SSB        52
51 NMAX=NMAX+10  Next region not sharp shock                       SSB        53
   CALL JMNMX(NMAX)                                                SSB        54
   RETURN                                                          SSB        55
   END                                                             SSB        56
```

SSB

Calculates the decomposition of an HE using a sharp shock model. All of the HE is burned at the shock front.

Local Variables

II = IE(I) = original region #.

ISSB = index incremented by one each cycle to keep track of when a cell should be burned.

Notes

The sharp shock burn runs with the following constraints on the cell at the shock front.

1. The inside boundary is held at a fixed position.
2. The outside boundary is moved at the CJ particle velocity.
3. The viscosity and pressure are set to zero until the cell is burned.
4. The cell is compressed for the time it takes for the wave to cross the cell at the detonation velocity. (The time step is set so that this takes four cycles.)
5. When the cell is burned, the internal energy and pressure are set on the Hugoniot for that volume.

For converging geometry the detonation velocity and particle velocity are no longer constant. The first cell is burned with the slab geometry values and the rest are calculated with a new detonation velocity D_{CJ}, particle velocity U_{CJ}, and time step Δt that are calculated from

$$D_{CJ} = V_0[P_{CJ}/(V_0 - V_{CJ})]^{0.5} \quad , \tag{1}$$

$$U_{CJ} = -[P_{CJ}(V_0 - V_{CJ})]^{0.5} \quad , \tag{2}$$

$$\Delta t = (\Delta X/D_{CJ})0.25 \quad , \tag{3}$$

where

P_{CJ} = Hugoniot P, V_{CJ} = V of cell just burned.

When the shock arrives at a new explosive, the new input CJ detonation and particle velocities are used to compress the new explosive.

The advantages of a sharp shock burn are that one can obtain excellent Taylor waves by using a small number of cells to describe multiple layers of explosives in plane or converging geometry. The disadvantages are that it requires more information and more artificial constraints than do the CJ volume or Arrhenius-burn techniques. The sharp shock burn can give incorrect results for systems in diverging geometry and for systems that are overdriven or significantly underdriven.

```
      SUBROUTINE FOREST(I)                                                  FOREST     2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,             PARAM      2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                      PARAM      3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                        PARAM      4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                            PARAM      5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                             MCELL      2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)       MCELL      3
     +,W(MCL)                                                               MCELL      4
      LEVEL 2,R                                                             MCELL      5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM,     MCELL      6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                        MCELL      7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                      MCELL      8
      LEVEL 2,TIME                                                          MCELL      9
      COMMON/INIT/DTD(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO     INIT       2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML),    INIT       3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)                INIT       4
      COMMON/BRND/Z(ML),E(ML),VCJ(ML),DWDT(NDW,ML),PCJ(ML),PM(ML),ND(ML)    BRD        2
     +,MSFF                                                                 BRD        3
      COMMON/MNMX/KMAX(ML2),KMIN(ML2),NMC                                   MN         2
      COMMON/ES/IE(ML2),NME                                                 ESM        2
      II=IE(I)                                                              FOREST     9
      JMN=JMIN(I)                                                           FOREST    10
      JMX=JMAX(I)                                                           FOREST    11
      JL=JMN                                                                FOREST    12
      DO 10 J=JMN,JMX                                                       FOREST    13
      IF(W(J).LE.0.) GO TO 11  All burned                                   FOREST    14
      PPQ=P(J)+AMAX1(0.,Q(J))  Pressure dependent rate                      FOREST    15
      IF(PPQ.LT.PM(II)) GO TO 10  Minimum pressure to calculate burn        FOREST    16
      IF(PPQ.GT.PCJ(II)) GO TO 11  Burn all if PPQ > PCJ                    FOREST    17
      IF(MSFF.EQ.0)GO TO 20  Multiple shock Forest Fire?                    FOREST    18
      IF(SX(J).NE.0.)GO TO 21  Has 1st shock passed?                        FOREST    19
      IF(J.NE.JMX)GO TO 22  Special at JMX for reflected shocks             FOREST    20
      JP=JMIN(I+1)                                                          FOREST    21
      PP=P(JP)+AMAX1(0.,Q(JP))   If the pressure in the next material exceeds FOREST  22
      IF(PP.LT.SX(JL))GO TO 22   that in the nearest cell flagged as the    FOREST    23
      DO 33 JJ=JL,JMX            shock having passed, then those cells not  FOREST    24
   33 SX(JJ)=SX(JL)              flagged as the shock having passed are flagged FOREST 25
      GO TO 21                   with that pressure in SX.                  FOREST    26
   22 CONTINUE                                                              FOREST    27
      PQL=SZ(J)  P + Q from previous cycle is in SZ                         FOREST    28
      SZ(J)=PPQ                                                             FOREST    29
      IF(PPQ.GT.PQL)GO TO 20                                                FOREST    30
      SX(J)=PPQ  Shock has passed; set SX                                   FOREST    31
   21 CONTINUE                                                              FOREST    32
      JL=J                                                                  FOREST    33
      IF(PPQ.LT.SX(J))SX(J)=PPQ  Pressure used to determine rate, may decrease FOREST 34
      PPQ=SX(J)                                        but not increase     FOREST    35
   20 CONTINUE                                                              FOREST    36
      SUM=0.                                                                FOREST    37
      NDA=ND(II)                                                            FOREST    38
      DO 1000 N=1,NDA                                                       FOREST    39
 1000 SUM=SUM*PPQ+DWDT(N,II)  Polynomial fit                                FOREST    40
      IF(SUM.GT.100.)SUM=100.  Avoid overflow                               FOREST    41
      RATE=EXP(SUM)  Rate                                                   FOREST    42
      W(J)=W(J)*(1.-DT*RATE)  New W                                         FOREST    43
      IF(W(J).LT.0.05) W(J)=0.                                              FOREST    44
      GO TO 10                                                              FOREST    45
   11 W(J)=0.                                                               FOREST    46
10    CONTINUE                                                             FOREST    47
      RETURN                                                                FOREST    48
      END                                                                   FOREST    49
```

FOREST(I)

Calculates the decomposition using the Forest Fire burn model. This model is appropriate for cases that require a non-negligible distance of run to detonation for the given input shock strength.

Local Variables

II = IE(I) = original region #.

JMN = minimum cell #.

JMX = maximum cell #.

J = do loop index = cell #.

PPQ = P + Max (Q,0).

SUM = temporary variable used to sum the $A_n P^n$ terms in the rate fit.

NDA = # of rate constants = n + 1.

RATE = $-\frac{1}{W}\frac{dW}{dt}$ from the fit.

Notes

This discussion of the Forest Fire rates is a condensed version of Appendix B in LA-7245. An even more thorough discussion of Forest Fire is in LA-6259. Several assumptions are made: (1) the Pop plot (ℓn P vs ℓn run of distance to detonation) is a straight line given by

$$\ell n\ (run) = a_1 + a_2\ \ell n\ (P - a_3) \quad . \tag{1}$$

where a_1, a_2, and a_3 are constants depending on the HE, and P is the input shock pressure; (2) the "single-curve buildup hypothesis" that the pressure grows along a unique line in (time, distance, state) space during buildup to detonation and that the Pop plot gives that line; (3) the "reactive Hugoniot" is assumed to be described by a USUP fit (several USUP fits are allowed but are not treated in this derivation)

$$U_S = C + SU_P \quad , \tag{2}$$

which gives from the jump conditions for $P_0 = 0$,

$$P = \rho_0 U_S U_P \quad , \tag{3}$$

$$V = V_0(U_S - U_P)/U_S \quad , \tag{4}$$

$$I = U_P^2/2 \quad ; \tag{5}$$

(4) the HOM EOS is used with the functional form

$$P = H(V,I,W) \quad . \tag{6}$$

The Lagrange coordinates m,τ are related to the Eulerian coordinates x,t by

$$\frac{\partial}{\partial m} = \frac{1}{\rho}\frac{\partial}{\partial x} \tag{7}$$

and

$$\frac{\partial}{\partial \tau} = \frac{\partial}{\partial t} + U\frac{\partial}{\partial x} \quad . \tag{8}$$

Letting subscripts denote partial derivatives with respect to the subscript, the fluid flow equations are

$$U_\tau = -P_m \quad , \tag{9}$$

$$V_\tau = U_m \quad , \tag{10}$$

and

$$I_\tau = -PV_\tau \quad . \tag{11}$$

The derivatives of shock front quantities are denoted by the symbol °. The equations for these derivatives are

$$\mathring{P} \equiv \frac{dP(x_s(t),t)}{dt} = P_m m_\tau + P_\tau = \rho_0 U_S P_m + P_\tau = \frac{dP}{d_{run}} U_S \quad , \tag{12}$$

where $x_s(t)$ is the shock position, and

$$\mathring{U} = \rho_0 U_S U_m + U_\tau = \frac{dU}{dP}\frac{dP}{dt} = \frac{\mathring{P}V_0}{C + 2SU} \quad . \tag{13}$$

Finally, the total derivative of the equation is given by

$$P_\tau = H_V V_\tau + H_I I_\tau + H_W W_\tau \quad , \tag{14}$$

which can be solved for W_τ, the desired quantity.

The usual calculation is for W_τ as a function of pressure. The pressure-dependent rate has proved useful, but there is nothing in the calculation that says the rate is a function of pressure only. The solutions are for rates on the Hugoniot and any variable will do (P, T, V, or I). Once off the Hugoniot, assumptions about what variable (or variables) determine the rate leads to different rates for a given state. For this derivation we will assume the rate is a function of pressure only.

Given P, the run is given by Eq. (1). The particle velocity can be obtained using Eq. (2) and Eq. (3) to give

$$U_P = \frac{-\rho_0 C + \sqrt{(\rho_0 C)^2 + 4P\rho_0 S}}{2\rho_0 S} \quad . \tag{15}$$

We have U_S from Eq. (2) and Eq. (5). Having U_S and U_P, we substitute in Eq. (4) and Eq. (5) to get V and I. Then, knowing P, V, and I, we solve P = H(V,I,W) for W. Now, with V, I, and W, we calculate the derivatives H_V, H_I, and H_W at that state point.

The shock front derivatives can be calculated using Eq. (1), Eq. (12), Eq. (13), and the already calculated value of U_P. The usual assumption $P_m = 0$ is then made. Eq. (12) becomes

$$P_\tau = \mathring{P} \tag{16}$$

and Eq. (13) combines with Eq. (9) and Eq. (10) to give

$$V_\tau = \frac{\mathring{U}}{\rho_0 U_S} \quad . \tag{17}$$

We already know I_τ from Eq. (11). Using the known values of P_τ, H_V, H_τ, H_I, I_τ, and H_W, we have

$$W_\tau(P) = \frac{H_V V_\tau + H_I I_\tau - P_\tau}{H_W} \quad . \tag{18}$$

The function $\ell n\ (-\frac{1}{W} W_\tau)$ is then fit to a polynomial of the form

$$\ell n \left(-\frac{W_\tau}{W}\right) \cong \sum_{i=0}^{n} A_i P^i \quad . \tag{19}$$

The constants DWDT(N,II) are related to the A_i's by

$$\text{DWDT(N,II)} = A_{n-(N-1)} \cdot \tag{20}$$

The value of P + Q (denoted PPQ) is used instead of P to calculate the rate. The fluid flow equations are solved using P + Q instead of P, so this is consistent. If PPQ < PM(II), then the rate would be so small it would not be worthwhile to calculate it. If PPQ > PCJ(II), where PCJ is the CJ pressure, then the cell is all burned. For W < 0.05 the cell is also all burned. Except for the above restrictions, the new mass fraction is given by

$$W_{new} = W_{old}\left(1 - \Delta t \exp\left(\sum_{i=0}^{n} A_i (P + Q)^i\right)\right) \quad , \tag{21}$$

which is a linearized version of

$$\Delta W = W_{new} - W_{old} = \int_{t_{old}}^{t_{new}} W(-\frac{1}{W} W_\tau)\, d\tau \ , \qquad (22)$$

with $\ell n \left(-\frac{W_\tau}{W}\right)$ replaced by the fit.

```
      SUBROUTINE FFT(I)                                                 FFT         2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM       2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM       3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM       4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                        PARAM       5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                         MCELL       2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)   MCELL       3
     +,W(MCL)                                                           MCELL       4
      LEVEL 2,R                                                         MCELL       5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM, MCELL       6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                    MCELL       7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                  MCELL       8
      LEVEL 2,TIME                                                      MCELL       9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO  INIT        2
     +(ML),TO(ML),RDW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT        3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)            INIT        4
      COMMON/BRND/Z(ML),E(ML),VCJ(ML),DWDT(NDW,ML),PCJ(ML),PM(ML),ND(ML) BRD       2
     +,MSFF                                                             BRD         3
      COMMON/ES/IE(ML2),NME                                             ESM         2
      II=IE(I)                                                          FFT         8
      JMN=JMIN(I)                                                       FFT         9
      JMX=JMAX(I)                                                       FFT        10
      DO 10 J=JMN,JMX                                                   FFT        11
      IF(W(J).LE.0.)GO TO 11   All burned                               FFT        12
      TP=T(J)  Temperature-dependent rate                               FFT        13
      IF(TP.LT.PM(II))GO TO 10   Minimum temperature to calculate burn  FFT        14
      IF(TP.GT.PCJ(II))GO TO 11  Burn it all                            FFT        15
      SUM=0.                                                            FFT        16
      NDA=ND(II)                                                        FFT        17
      DO 1000 N=1,NDA                                                   FFT        18
 1000 SUM=SUM*TP+DWDT(N,II)  Polynomial fit                             FFT        19
      IF(SUM.GT.100.)SUM=100.   Avoid overflow                          FFT        20
      RATE=EXP(SUM)   Rate                                              FFT        21
      W(J)=W(J)*(1.-DT*RATE)  New W                                     FFT        22
      IF(W(J).LT.0.05)W(J)=0.                                           FFT        23
      GO TO 10                                                          FFT        24
   11 W(J)=0.                                                           FFT        25
   10 CONTINUE                                                          FFT        26
      RETURN                                                            FFT        27
      END                                                               FFT        28
```

FFT

The Forest Fire rate is calculated as a function of temperature.

Local Variables

See FOREST.

Notes

The minimum temperature to calculate the rate is stored in PM and maximum temperature at which W is set to zero is stored in PCJ.

FFI

The Forest Fire rate is calculated as a function of specific internal energy.

Local Variables

See FOREST.

Notes

The minimum specific internal energy to calculate the rate is stored in PM and maximum temperature at which W is set to zero is stored in PCJ.

```
      SUBROUTINE FFI(I)                                                 FFI         2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM       2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM       3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM       4
     +,NSM=4,NWPM=3729,NSD=NSM*NWPM+132,ML2=100)                        PARAM       5
      COMMON/CELL/P(MCL),U(MCL),V(MCL),XI(MCL),                         MCELL       2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)   MCELL       3
     +,W(MCL)                                                           MCELL       4
      LEVEL 2,R                                                         MCELL       5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM, MCELL       6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                    MCELL       7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                  MCELL       8
      LEVEL 2,TIME                                                      MCELL       9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO  INIT        2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT        3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)            INIT        4
      COMMON/BRND/Z(ML),E(ML),VCJ(ML),DWDT(NDW,ML),PCJ(ML),PM(ML),ND(ML) BRD       2
     +,MSFF                                                             BRD         3
      COMMON/ES/IE(ML2),NME                                             ESM         2
      II=IE(I)                                                          FFI         8
      JMN=JMIN(I)                                                       FFI         9
      JMX=JMAX(I)                                                       FFI        10
      DO 10 J=JMN,JMX                                                   FFI        11
      IF(W(J).LE.0.)GO TO 11  All burned                                FFI        12
      E=XI(J)   Internal energy-dependent rate                          FFI        13
      IF(E.LT.PM(II))GO TO 10  Minimum energy to calculate rate         FFI        14
      IF(E.GT.PCJ(II))GO TO 11  Burn it all                             FFI        15
      SUM=0.                                                            FFI        16
      NDA=ND(II)                                                        FFI        17
      DO 1000 N=1,NDA                                                   FFI        18
 1000 SUM=SUM*E+DWDT(N,II)   Polynomial fit                             FFI        19
      IF(SUM.GT.100.)SUM=100.   Avoid overflow                          FFI        20
      RATE=EXP(SUM)  Rate                                               FFI        21
      W(J)=W(J)*(1.-DT*RATE)  New W                                     FFI        22
      IF(W(J).LT.0.05)W(J)=0.                                           FFI        23
      GO TO 10                                                          FFI        24
   11 W(J)=0.                                                           FFI        25
   10 CONTINUE                                                          FFI        26
      RETURN                                                            FFI        27
      END                                                               FFI        28
```

```
      SUBROUTINE GLTW(I)                                                GLTW      2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM     2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM     3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM     4
     +,NSM=4,NWPM=372R,NSD=NSM*NWPM+132,ML2=100)                        PARAM     5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                         MCELL     2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)   MCELL     3
     +,W(MCL)                                                           MCELL     4
      LEVEL 2,R                                                         MCELL     5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM, MCELL     6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                    MCELL     7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                  MCELL     8
      LEVEL 2,TIME                                                      MCELL     9
      COMMON/BUX/BUA,BUR,BUMAX,BUDV(ML)                                 BUP       2
     +,BUR,BUD                                                          BUP       3
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO INIT      2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT      3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)            INIT      4
      COMMON/ES/IE(ML2),NME                                             ESM       2
      COMMON/MNMX/KMAX(ML2),KMIN(ML2),NMC                               MN        2
      COMMON/EOSN/IEOS(ML),ME(ML)                                       EN        2
      COMMON/GASC/GC(NGC,ML)                                            GC        2
      COMMON/BRND/Z(ML),E(ML),VCJ(ML),DWDT(NDW,ML),PCJ(ML),PM(ML),ND(ML) BRD      2
     +,MSFF                                                             BRD       3
      COMMON/UCJC/X1,I1,NMAX,X2,X3                                      GLTW     12
      II=IE(I)                                                          GLTW     13
      JMN=JMIN(I)                                                       GLTW     14
      JMX=JMAX(I)                                                       GLTW     15
      RO=R(JMX+1)                                                       GLTW     16
      G=GC(2,II)                                                        GLTW     17
      IF(IEOS(II).EQ.2)G=T(JMX)                                         GLTW     18
      GP=G+1                                                            GLTW     19
      GM=G-1                                                            GLTW     20
      DV=VCJ(II)                                                        GLTW     21
      IF(IEOS(II).EQ.2)DV=SQRT(BUDV(II))                                GLTW     22
      DV2=DV*DV                                                         GLTW     23
      UCJ=DV/GP                                                         GLTW     24
      DRO=R(JMN)-R(JMN+1)                                               GLTW     25
      UL=-UCJ*GP/GM                                                     GLTW     26
      U(JMX+1)=-UCJ    Start with CJ conditions at shock front and calculate outward GLTW 27
      PCJ=DV2*ROW(II)/GP                                                GLTW     28
      CJV=G/(GP*ROW(II))                                                GLTW     29
      CCJ=UCJ*G                                                         GLTW     30
      DLR=V(JMX)*XM(JMX)                                                GLTW     31
      IF(IA.NE.0)DLR=DLR/(R(JMX+1)**IA)    Get new radius from V and M  GLTW     32
      R(JMX)=R(JMX+1)+DLR                                               GLTW     33
      DR=R(JMN)-RO                                                      GLTW     34
      DT=DR/DV                                                          GLTW     35
      J=JMX+1                                                           GLTW     36
      DO 10 JJ=JMN,JMX    Calculate cell quantities starting with the inside GLTW 37
      J=J-1                                                             GLTW     38
      W(J)=0.    All burned                                             GLTW     39
      U(J)=UCJ*(2*(R(J)-RO)/DR-1)                                       GLTW     40
      IF(U(J).GT.UF)U(J)=UF    Particle velocity                        GLTW     41
      CC=-GM*(U(J+1)+UL)/(2*G*UCJ)    Local C                           GLTW     42
      P(J)=PCJ*CC**(2*G/GM)                                             GLTW     43
      V(J)=CJV*CC**(-2/GM)    P,V,I solutions for that cell             GLTW     44
      XI(J)=P(J)*V(J)/GM-DV2/(2*GP*GM)                                  GLTW     45
      DLR=V(J)*XM(J)                                                    GLTW     46
      IF(IA.NE.0)DLR=DLR/(R(J)**IA)    Get new radius from V and M      GLTW     47
```

```
      R(J-1)=R(J)+DLR                                                    GLTW      48
   10 CONTINUE                                                           GLTW      49
      IF(J.NE.2)GO TO 11                                                 GLTW      50
      R(1)=R(2)                                                          GLTW      51
      U(1)=U(2)    Piston conditions if the HE was in region 1           GLTW      52
      BU=UF                                                              GLTW      53
      TIME=TIME+DT   Set the time to include the GLTW detonation time    GLTW      54
   11 CONTINUE                                                           GLTW      55
      IBRN(II)=1                                                         GLTW      56
      IF(I.EQ.1)RETURN                                                   GLTW      57
      NMAX=JMAX(I-1)   Special for other materials outside GLTW HE       GLTW      58
      CALL JMNMX(NMAX)                                                   GLTW      59
      NCI=JMX-JMN+1                                                      GLTW      60
      NT=NCI*12*(R(NMAX-1)-R(NMAX))/DRO                                  GLTW      61
      DT=DT/NT   Set time step                                           GLTW      62
      NCLT=NCL                                                           GLTW      63
      NCL=NMAX                                                           GLTW      64
      BUI=UF   Effect of HE treated as a piston                          GLTW      65
      KMAX(I-1)=KMAX(I-1)+1                                              GLTW      66
      NMC=I-1                                                            GLTW      67
      DO 20 II=1,NT                                                      GLTW      68
      TIME=TIME+DT    Run hydro for the outside regions to catch up with GLTW HE  GLTW  69
      CALL DIFEQ                                                         GLTW      70
   20 CONTINUE                                                           GLTW      71
      NCL=NCLT                                                           GLTW      72
      BUI=0.   Get rid of piston                                         GLTW      73
      KMAX(I-1)=KMAX(I-1)-1                                              GLTW      74
      NMAX=NMAX+NCI+3    Set up for normal hydro                         GLTW      75
      CALL JMNMX(NMAX)                                                   GLTW      76
      RETURN                                                             GLTW      77
      END                                                                GLTW      78
```

GLTW

An entire region of explosive is burned using the gamma-law Taylor-wave description.

Local Variables

CC = C in notes = sound speed.

CJV = V_{CJ} in notes = CJ volume.

DLR = width of a cell computed from its mass and specific volume.

DR = ΔR in notes = width of region.

DV = D in notes = detonation velocity.

DV2 = D^2.

G = γ in notes.

GM = $\gamma - 1$.

GP = $\gamma + 1$.

II = IE(I) = original region #.

J = cell # being computed.

JJ = do loop index.

JMN = JMIN(I).

JMX = JMAX(I).

NCI = # of cells in the first region outside the GLTW HE.

NCLT = temporary storage of NCL.

NT = # of time steps used to allow the first region outside the GLTW HE to respond.

RO = inside radius of the GLTW HE.

UCJ = U_{CJ} in notes = CJ particle velocity.

UL = $-U_{CJ}\left(\frac{\gamma + 1}{\gamma - 1}\right)$.

Notes

Following Fickett and Davis, we will outline the gamma-law Taylor-wave solution for a detonation. The equation of state in a rarefaction wave following the detonation is restricted to the CJ isentrope. The pressure and sound speed are then functions of density only. For a γ-law gas they are given by

$$P = P_{CJ}\left(\frac{V_{CJ}}{V}\right)^{\gamma} \tag{1}$$

and

$$C = C_{CJ}\left(\frac{P}{P_{CJ}}\right)^{(\gamma-1)/2\gamma} = \left(\frac{dP}{d\rho}\right)^{1/2} . \tag{2}$$

With the addition of two characteristic equations,

$$\frac{dP}{du} = \rho C \tag{3}$$

and

$$U + C = x/t \quad , \tag{4}$$

a solution can be found for $U(x/t)$ where x is the Eulerian distance and t is the time. From the jump conditions the CJ state has the following relations.

$$U_{CJ} = \frac{D}{\gamma + 1} \tag{5}$$

$$P_{CJ} = \frac{\rho_0 D^2}{\gamma + 1} \tag{6}$$

and

$$V_{CJ} = \frac{V_0 \gamma}{\gamma + 1} \quad . \tag{7}$$

Using Eqs. (1) and (2), we can solve Eq. (3) for

$$P = P_{CJ}\left[\frac{1 + (\gamma - 1)(U - U_{CJ})}{2C_{CJ}}\right]^{2\gamma/\gamma-1} . \tag{8}$$

Combining Eqs. (2), (4), and (8), we have

$$U = \left(\frac{2}{\gamma + 1}\right)\left(\frac{x}{t}\right) - U_{CJ} \quad . \tag{9}$$

By integrating the PdV work from infinite volume, one can find the specific internal energy on the CJ isentrope to be

$$I = \frac{P_V}{\gamma - 1} - \frac{P_{CJ}V_{CJ}}{\gamma - 1} + \frac{P_{CJ}}{2}(V_0 - V_{CJ}) \quad , \tag{10}$$

where the last term sets the zero of energy relative to the solid. The time is then set to

$$t = \frac{\Delta R}{D} \quad , \tag{11}$$

where ΔR is the width of the γ-law explosive. That is, the state is evaluated when the detonation has just crossed the entire region. For a given cell, we can use Eqs. (1), (8), (9), (10), and (11) to find V, P, U, and I. Then, from the mass and V, the radius of the inside of the next cell can be evaluated. For U greater than UF, the final piston velocity U is reset to the final piston velocity with the corresponding values for V, P, and I.

It must be remembered that Eq. (1) is the equation of state only on the CJ isentrope. Provision is made for either the HOM EOS or the Buildup EOS for subsequent evaluation of the EOS. However, the buildup EOS must not be used when the region is thick enough to require a nonconstant γ.

The GLTW is useful for burning a large region of HE in slab geometry with a minimum of computation. However, it has also proved useful in cylindrical or spherical geometry under certain restrictions. Since GLTW is designed for slab geometry, it can only be used for a small enough region that convergence

can be ignored. This small region can be used instead of a piston to initiate HE burn for a larger region. In some cases the usual piston initiation can be sufficiently zoning-dependent to be noticeable. By burning three cells of a large HE region using GLTW, the zoning dependence is minimal.

Provision is made for materials outside the GLTW HE. A separate calculation is made for the outside regions for the total detonation time of the GLTW HE. A piston with the final piston velocity UF acts on the outside regions from the inside.

```
      SUBROUTINE BNDR1                                                  BNDR1      2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM      2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM      3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM      4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                        PARAM      5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                         MCELL      2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)   MCELL      3
     +,W(MCL)                                                           MCELL      4
      LEVEL 2,R                                                         MCELL      5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM, MCELL      6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                    MCELL      7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                  MCELL      8
      LEVEL 2,TIME                                                      MCELL      9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO  INIT       2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT       3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)            INIT       4
      COMMON/VOID/INTX(ML2),JV(ML2),IV(ML2),NNV                         VD         2
      COMMON/MNMX/KMAX(ML2),KMIN(ML2),NMC                               MN         2
      COMMON/UCJC/UCJ,JJ,NMAX,RCJ,DCJ                                   UC         2
      COMMON/NSPLT/NOSPLT(ML2)                                          NSP        2
      COMMON/PWORK/PW,PWI                                               PWORK      2
      COMMON/ES/TE(ML2),NME                                             ESM        2
      COMMON/SPC/SP(ML),USP(ML)                                         SPLC       2
     +,XISP(ML)                                                         SPLC       3
      DATA IFLP/0/,IFLPI/0/                                             BNDR1     13
      IF(IBRN(NMC).NE.3)GO TO 20                                        BNDR1     14
      IF(JJ.LE.2)GO TO 20                                               BNDR1     15
      RCJ=RCJ+DT*UCJ          Sharp shock burn                          BNDR1     16
      R(JJ)=RCJ                                                         BNDR1     17
      U(JJ)=UCJ                                                         BNDR1     18
   20 CONTINUE                                                          BNDR1     19
      IFLP=IFLP-1                                                       BNDR1     20
      IFLPI=IFLPI-1                                                     BNDR1     21
      IF(BU.EQ.0.) GO TO 1   Skip if no outside piston                  BNDR1     22
      RO=R(1)                                                           BNDR1     23
      R(1)=R(1)+DT*BU         Outside piston boundary condition         BNDR1     24
      U(1)=BU                                                           BNDR1     25
      R(2)=R(1)                                                         BNDR1     26
      DVP=F2*0.5*(R(1)-RO)*(R(1)**IA+RO**IA+F3*R(1)*RO)                 BNDR1     27
      PW=PW+(P(2)+Q(2))*DVP   Work done by the piston                   BNDR1     28
      IF(IFLP.LT.0)PW=PW+XM(2)*((U(2)+U(3))**2-(U(1)+U(3))**2)          BNDR1     29
      IFLP=1                                                            BNDR1     30
      U(2)=U(1)                                                         BNDR1     31
    1 CONTINUE                                                          BNDR1     32
      IF(BUI.EQ.0.)GO TO 11   Skip if no inside piston                  BNDR1     33
      RO=R(NCL+1)                                                       BNDR1     34
      R(NCL+1)=R(NCL+1)+DT*BUI  Inside piston boundary condition        BNDR1     35
      U(NCL+1)=BUI                                                      BNDR1     36
      IF(R(NCL).GT.R(NCL+1))GO TO 11                                    BNDR1     37
      R(NCL)=R(NCL+1)                                                   BNDR1     38
      DVPI=F2*0.5*(R(NCL)-RO)*(R(NCL)**IA+RO**IA+F3*R(NCL)*RO)          BNDR1     39
      PWI=PWI+(P(NCL)+Q(NCL))*DVPI  Work done by piston                 BNDR1     40
      IFLPI=1                                                           BNDR1     41
      U(NCL)=U(NCL+1)                                                   BNDR1     42
   11 CONTINUE                                                          BNDR1     43
      IF(R(NCL).GT.1.E-10.OR.IA.EQ.0) GO TO 5 Special for converging geometry BNDR1 44
      R(NCL)=1.E-10  If R(NCL) is 0, the difference equations won't allow it to move BNDR1 45
      NOSPLT(NM)=0  Don't rezone after R(NCL) hits the origin           BNDR1     46
      U(NCL)=0.   Don't move until it goes into tension                 BNDR1     47
    5 CONTINUE                                                          BNDR1     48
```

```
      IF(NNV.EQ.0)RETURN   Skip if no voids                                  BNDR1   49
      DO 2 I=1,NMC                                                           BNDR1   50
      IF(IV(I).LT.0) GO TO 2   No void                                       BNDR1   51
      J=JV(I)                                                                BNDR1   52
      IF(J.GT.JMAX(NMC)) GO TO 2  Void not active                            BNDR1   53
      IF(IV(I).GE.1)GO TO 3  Go check for closed void in tension             BNDR1   54
      IF(R(J).GT.R(J+1))GO TO 2  Open void still open                        BNDR1   55
      DU=U(J)-U(J+1)   Void closes with relative velocity DU                 BNDR1   56
      PRINT 100,TIME,R(J),DU,I,J,MAT(I),MAT(I+1)                             BNDR1   57
      WRITE(8,100)TIME,R(J),DU,I,J,MAT(I),MAT(I+1)                           BNDR1   58
  100 FORMAT(21H1VOID COLLAPSE: TIME=,1PE12.5,8H RADIUS=,1PE12.5,            BNDR1   59
     +4H DU=,1PE12.5,3H I=,I3,3H J=,I5,17H MATERIAL NUMBERS,2I6)             BNDR1   60
      IF(DU.LT.-0.5)GO TO 4  Special treatment for high velocity             BNDR1   61
      DR=R(J)-R(J+1)                                                         BNDR1   62
      R(J)=(R(J)+R(J+1))/2                                                   BNDR1   63
      R(J+1)=R(J)          Calculate R,U for newly closed interface          BNDR1   64
      U(J)=(U(J)+U(J+1))/2  as if materials are the same                     BNDR1   65
      U(J+1)=U(J)                                                            BNDR1   66
      IV(I)=1   Closed void flag                                             BNDR1   67
      GO TO 2                                                                BNDR1   68
    4 CALL RL(I)   Special treatment for high velocity                       BNDR1   69
      IV(I)=2                                                                BNDR1   70
      GO TO 2                                                                BNDR1   71
    3 II=IE(I)                                                               BNDR1   72
      IF(P(J+1).LT.XISP(II).AND.P(J-1).LT.XISP(II))IV(I)=0  Open void?        BNDR1   73
      IF(IV(I).EQ.0)PRINT 101,TIME,R(J),I,J,MAT(I),MAT(I+1)                  BNDR1   74
      IF(IV(I).EQ.0)WRITE(8,101)TIME,R(J),I,J,MAT(I),MAT(I+1)                BNDR1   75
  101 FORMAT(18H1VOID OPENS: TIME=,1PE12.5,8H RADIUS=,1PE12.5,               BNDR1   76
     +3H I=,I3,3H J=,I5,17H MATERIAL NUMBERS,2I6)                            BNDR1   77
    2 CONTINUE                                                               BNDR1   78
      RETURN                                                                 BNDR1   79
      ENTRY BNDR2                                                            BNDR1   80
      IF(IFLP.EQ.1)PW=PW+(P(2)+Q(2))*DVP          Work done by pistons       BNDR1   81
      IF(IFLPI.EQ.1)PWI=PWI+(P(NCL)+Q(NCL))*DVPI                             BNDR1   82
      RETURN                                                                 BNDR1   83
      END                                                                    BNDR1   84
```

BNDR1

Calculates several special boundary conditions such as an applied piston.

Local Variables

I = do loop index = region #.

J = JV(I) = cell# for outside free surface of open void.

DU = relative velocity of the two free surfaces bounding an open void.

DR = position difference of the two free surfaces bounding a just closed void. The positions were calculated assuming the void would not close.

Notes

For sharp-shock burn, the cell currently being burned has its outside cell boundary moving at the computed CJ particle velocity instead of the results of hydrodynamics. A piston on the inside of the problem and a piston on the outside of the problem are allowed. (Pistons are only calculated when their velocity is not set to 0.) Piston positions are calculated using the input piston velocities BU and BUI. The inside and outside radii of the problem are calculated assuming they are free surfaces. If a radius is not within the limits of the corresponding piston then it is reset to the piston value and the velocity is reset to the piston velocity. For spherical and cylindrical geometry the origin cannot be crossed (yielding negative radii?). If it is, the inside radius is reset to 10^{-10}. A negligible but positive value is used in order to allow the inside surface to move under tension. Otherwise, the difference equations will not allow it to move under any circumstances. Also, a flag is reset to turn off rezoning for the inside region after the inside surface hits the origin.

If there are voids, a check is made whether an open void just closed or a closed void should open. A closed void is allowed to open under tension.

When a void closes, the two free surfaces "overshoot" each other. An extrapolation is made back to the point of contact. The two velocities are reset to the average velocity. This velocity is correct only for identical materials. However, the difference equations will bring the interface velocity to its proper value unless the relative velocity is too great. For large relative velocities, the artificial viscosity treatments currently in use in the code will dump too much internal energy into the cells bounded by the interface before the cell boundaries have time to respond. That is, the difference in velocity across a cell next to a just-closed interface becomes instantaneously finite. When this difference is large (and viscosity depends on this difference in velocity) the above-mentioned problem occurs. A special treatment is made in this case that is described in RL.

```
      SUBROUTINE SL(I)                                                  SL          2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM       2
     +NUMV=10,MOL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM       3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM       4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                        PARAM       5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                         MCELL       2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)   MCELL       3
     +,W(MCL)                                                           MCELL       4
      LEVEL 2,R                                                         MCELL       5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM, MCELL       6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                    MCELL       7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                  MCELL       8
      LEVEL 2,TIME                                                      MCELL       9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO  INIT        2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT        3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)            INIT        4
      COMMON/VOID/INTX(ML2),JV(ML2),IV(ML2),NNV                         VD          2
      COMMON/MNMX/KMAX(ML2),KMIN(ML2),NMC                               MN          2
      COMMON/NSPLT/NOSPLT(ML2)                                          NSP         2
      COMMON/ES/IE(ML2),NME                                             ESM         2
      IPM=NM+1                                                          SL         10
      J=JS   Cell # to spall                                            SL         11
      IF(IPM.GE.ML2)RETURN   Don't make more regions than storage allows SL        12
      II=IE(I)                                                          SL         13
      CALL OUTGAS   GAS dump before spall                               SL         14
      PRINT 100,TIME,R(J),I,J,MAT(II)                                   SL         15
      WRITE(8,100)TIME,R(J),I,J,MAT(II)                                 SL         16
  100 FORMAT(13H1SPALL: TIME=,1PE12.5,8H RADIUS=,1PE12.5,3H I=,I3,      SL         17
     +3H J=,I5,16H MATERIAL NUMBER,I6)                                  SL         18
      CALL PRNT  Print out before spall                                 SL         19
      DO 10 II=I,NM                                                     SL         20
      IP=IPM                                                            SL         21
      IPM=IP-1                                                          SL         22
      IE(IP)=IE(IPM)                                                    SL         23
      IV(IP)=IV(IPM)                                                    SL         24
      JV(IP)=JV(IPM)                                                    SL         25
      INTX(IP)=INTX(IPM)                                                SL         26
      JMAX(IP)=JMAX(IPM)    Shift variables that characterize the region up by 1 SL 27
      KMAX(IP)=KMAX(IPM)                                                SL         28
      JMIN(IP)=JMIN(IPM)                                                SL         29
      KMIN(IP)=KMIN(IPM)                                                SL         30
      NOSPLT(IP)=NOSPLT(IPM)                                            SL         31
   10 CONTINUE                                                          SL         32
      NM=NM+1     One new region                                        SL         33
      NMC=NMC+1                                                         SL         34
      CALL SHFT(I,J,1)   Shift cell quantities up by 1                  SL         35
      NNV=NNV+1  A new void                                             SL         36
      IV(I)=0      that is open                                         SL         37
      JP=J+1                                                            SL         38
      XM(J)=0.    Void cell                                             SL         39
      JV(I)=J                                                           SL         40
      IT=1                                                              SL         41
      IF(INTX(I).GE.2) IT=5   Set interface flag                        SL         42
      INTX(I)=IT                                                        SL         43
      JMAX(I)=J-1                                                       SL         44
      KMAX(I)=J-1                                                       SL         45
      JMIN(I+1)=JP   Set region boundaries                              SL         46
      KMIN(I+1)=JP                                                      SL         47
      NOSPLT(I)=0   Turn off rezoning                                   SL         48
      R(JP)=R(J)                                                        SL         49
```

```
      IFLAG(J)=IFLAG(J-1)+64
      JMN=JP
      JMX=KMAX(NM)
      DO 12 K=JMN,JMX
      IFLAG(K)=IFLAG(K)+128
   12 CONTINUE
      IFLAG(NCL)=IFLAG(NCL)+128
      CALL OUTGAS    GAS dump after spall
      JS=0    Turn off spall flag
      RETURN
      END
```

Set flags so that GAS plots will show spall on interface plots

SL 50
SL 51
SL 52
SL 53
SL 54
SL 55
SL 56
SL 57
SL 58
SL 59
SL 60

SL(I)

Does all the bookkeeping required to create a spall.

Local Variables

IPM = NM+1 = # of regions after the spall (which splits one region into two); also, IPM is decremented in the do loop where data is shifted.

J = JS = cell # to spall.

II = IE(I) = original region #; also do loop index.

IP = previous value of IPM in the do loop where data is shifted.

JP = J+1 = cell # next to the created void.

IT = temporary variable to calculate INTX.

Notes

When a spall occurs, a single region is split into two regions with an open void between them. The open void requires a new cell to be created.

```
      SUBROUTINE SPLTCHK                                                SPLTCHK    2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM      2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM      3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM      4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                        PARAM      5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                         MCELL      2
     +P(MCL),SX(MCL),SY(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)   MCELL      3
     +,W(MCL)                                                           MCELL      4
      LEVEL 2,R                                                         MCELL      5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UIT,UFT,NADD,NM, MCELL      6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                    MCELL      7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                  MCELL      8
      LEVEL 2,TIME                                                      MCELL      9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO  INIT       2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT       3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)            INIT       4
      COMMON/MNMX/KMAX(ML2),KMIN(ML2),NMC                               MN         2
      COMMON/NSPLT/NOSPLT(ML2)                                          NSP        2
      COMMON/ES/IE(ML2),NME                                             ESM        2
      DATA DRMN/0.001/                                                  SPLTCHK    9
      DATA N/4/                                                         SPLTCHK   10
      IF(KMAX(NM).GE.MCL-1-N)RETURN   Don't overrun storage             SPLTCHK   11
      DO 10 I=1,NMC                                                     SPLTCHK   12
      IF(NOSPLT(I).LE.0) GO TO 10   Is rezoning allowed?                SPLTCHK   13
      J=KMAX(I)                                                         SPLTCHK   14
      DLR=R(J)-R(J+1)                                                   SPLTCHK   15
      II=IE(I)                                                          SPLTCHK   16
      DR=5*DRO(II)        If the innermost cell has ΔR > 4ΔR0, then rezone SPLTCHK   17
      IF(DLR.LT.DR) GO TO 10                                            SPLTCHK   18
   12 CONTINUE                                                          SPLTCHK   19
      NCI=KMAX(I)-KMIN(I)+1                                             SPLTCHK   20
      IF(N.GT.NCI)N=NCI   Don't split cells outside the region          SPLTCHK   21
      CALL OUTGAS                                                       SPLTCHK   22
      CALL SHFT(I,J,N)   Shift cells inside of the split by N           SPLTCHK   23
   11 CALL SPLIT(I,J,N)  Split the last N cells in half                 SPLTCHK   24
      CALL PRNT                                                         SPLTCHK   25
      CALL OUTGAS                                                       SPLTCHK   26
   10 CONTINUE                                                          SPLTCHK   27
      RETURN                                                            SPLTCHK   28
      END                                                               SPLTCHK   29
```

SPLTCHK

Checks whether rezoning is required in a region and if so calls subroutines to do the rezoning.

Local Variables

N = # of cells to be split if rezoning is required.

I = do loop index = region #.

J = cell # of innermost cell in region I.

DLR = width of cell J.

DR = 5 times initial width of cell J.

NCI = # of cells in region I.

Notes

Rezoning is not checked for unless NOSPLT(I) > 0. Currently, the only criterion included is that the innermost cell of a region gets wider than five times the initial width. Other criteria are available for particular types of problems. The GAS dump before and after the rezoning is to avoid extraneous lines in certain types of plots.

```
      SUBROUTINE SHFT(I,J,N)                                                SHFT     2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,             PARAM    2
     +NUMV=10,MOL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                      PARAM    3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                        PARAM    4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                            PARAM    5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                             MCELL    2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)       MCELL    3
     +,W(MCL)                                                               MCELL    4
      LEVEL 2,R                                                             MCELL    5
      COMMON/DVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM,     MCELL    6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                        MCELL    7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                      MCELL    8
      LEVEL 2,TIME                                                          MCELL    9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO     INIT     2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML),    INIT     3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)                INIT     4
      COMMON/UCJC/UCJ,JJ,NMAX,RCJ,DCJ                                       UC       2
      COMMON/VOID/INTX(ML2),JV(ML2),IV(ML2),NNV                             VD       2
      COMMON/MNMX/KMAX(ML2),KMIN(ML2),NMC                                   MN       2
      JJ=NCL+1                                                              SHFT     9
      R(JJ+N)=R(JJ)                                                         SHFT    10
      U(JJ+N)=U(JJ)                                                         SHFT    11
      DO 10 K=J,NCL                                                         SHFT    12
      JJ=JJ-1                                                               SHFT    13
      JN=JJ+N                                                               SHFT    14
      R(JN)=R(JJ)                                                           SHFT    15
      U(JN)=U(JJ)                                                           SHFT    16
      P(JN)=P(JJ)                                                           SHFT    17
      V(JN)=V(JJ)          Shift cell quantities up by N for cell #'s > J   SHFT    18
      XI(JN)=XI(JJ)                                                         SHFT    19
      SX(JN)=SX(JJ)                                                         SHFT    20
      SZ(JN)=SZ(JJ)                                                         SHFT    21
      W(JN)=W(JJ)                                                           SHFT    22
      XM(JN)=XM(JJ)                                                         SHFT    23
      IFLAG(JN)=IFLAG(JJ)                                                   SHFT    24
      T(JN)=T(JJ)                                                           SHFT    25
      Q(JN)=Q(JJ)                                                           SHFT    26
   10 CONTINUE                                                              SHFT    27
      DO 11 K=I,NM                                                          SHFT    28
      KMAX(K)=KMAX(K)+N                                                     SHFT    29
      JMAX(K)=JMAX(K)+N    1st KMIN, KMAX, JMIN, JMAX reflect the shifted cells SHFT 30
      IF(I.EQ.K) GO TO 11                                                   SHFT    31
      JMIN(K)=JMIN(K)+N                                                     SHFT    32
      KMIN(K)=KMIN(K)+N                                                     SHFT    33
   11 CONTINUE                                                              SHFT    34
      DO 12 K=1,NM                                                          SHFT    35
   12 IF(JV(K).GT.J) JV(K)=JV(K)+N  Shift void cell index                   SHFT    36
      NCL=NCL+N            N new cells                                      SHFT    37
      NMAX=NMAX+N                                                           SHFT    38
      RETURN                                                                SHFT    39
      END                                                                   SHFT    40
```

SHFT

Shifts all cells with cell # $\geq$ J up by N. Used when new cells are created in the middle of the problem; e.g., for spall and rezoning.

Local Variables

JJ = index of cell being shifted.

JN = index of cell to which cell # JJ quantities are being shifted.

K = do loop index.

Notes

Any new quantities that are tied to a cell # should be included in this subroutine.

```
      SUBROUTINE SPLIT(I,J,N)                                           SPLIT     2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM     2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM     3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM     4
     +,NSM=4,NWPM=372A,NSD=NSM*NWPM+132,ML2=100)                        PARAM     5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                         MCELL     2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)   MCELL     3
     +,W(MCL)                                                           MCELL     4
      LEVEL 2,R                                                         MCELL     5
      COMMON/DVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM, MCELL     6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                    MCELL     7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                  MCELL     8
      LEVEL 2,TIME                                                      MCELL     9
      JJ=J+1                                                            SPLIT     5
      JP=J+N+1                                                          SPLIT     6
      R(JP)=R(JJ)                                                       SPLIT     7
      U(JP)=U(JJ)                                                       SPLIT     8
      DO 10 K=1,N                                                       SPLIT     9
      JP=JP-2                                                           SPLIT    10
      JJ=JJ-1                                                           SPLIT    11
      IFLAG(JP)=IFLAG(JJ)                                               SPLIT    12
      IFLAG(JP+1)=IFLAG(JJ)                                             SPLIT    13
      R(JP+1)=(R(JJ)+R(JJ+1))/2                                         SPLIT    14
      R(JP)=R(JJ)                                                       SPLIT    15
      U(JP+1)=(U(JJ)+U(JJ+1))/2                                         SPLIT    16
      U(JP)=U(JJ)                                                       SPLIT    17
      JM=JJ-1                                                           SPLIT    18
      XMF=0.5*XM(JJ)/(XM(JJ)+XM(JM))                                    SPLIT    19
      DV=XMF*(V(JJ)-V(JM))                                              SPLIT    20
      V(JP+1)=V(JJ)+DV                                                  SPLIT    21
      V(JP)=V(JJ)-DV                                                    SPLIT    22
      DV=XMF*(P(JJ)-P(JM))                                              SPLIT    23
      P(JP+1)=P(JJ)+DV                                                  SPLIT    24
      P(JP)=P(JJ)-DV                                                    SPLIT    25
      DV=XMF*(XI(JJ)-XI(JM))                                            SPLIT    26
      XI(JP+1)=XI(JJ)+DV                  Interpolate                   SPLIT    27
      XI(JP)=XI(JJ)-DV                      cell quantities             SPLIT    28
      DV=XMF*(SX(JJ)-SX(JM))                                            SPLIT    29
      SX(JP+1)=SX(JJ)+DV                                                SPLIT    30
      SX(JP)=SX(JJ)-DV                                                  SPLIT    31
      DV=XMF*(SZ(JJ)-SZ(JM))                                            SPLIT    32
      SZ(JP+1)=SZ(JJ)+DV                                                SPLIT    33
      SZ(JP)=SZ(JJ)-DV                                                  SPLIT    34
      DV=XMF*(W(JJ)-W(JM))                                              SPLIT    35
      W(JP+1)=W(JJ)+DV                                                  SPLIT    36
      W(JP)=W(JJ)-DV                                                    SPLIT    37
      DV=XMF*(T(JJ)-T(JM))                                              SPLIT    38
      T(JP+1)=T(JJ)+DV                                                  SPLIT    39
      T(JP)=T(JJ)-DV                                                    SPLIT    40
      DV=XMF*(Q(JJ)-Q(JM))                                              SPLIT    41
      Q(JP+1)=Q(JJ)+DV                                                  SPLIT    42
      Q(JP)=Q(JJ)-DV                                                    SPLIT    43
      CF=XM(JJ)                                                         SPLIT    44
      DR=R(JP+1)-R(JP+2)                                                SPLIT    45
      R1=R(JP+2)                                                        SPLIT    46
      R2=R(JP+1)                                                        SPLIT    47
      XM(JP+1)=DP*F2*(R1**IA+R2**IA+F3*R1*R2)/V(JP+1)                   SPLIT    48
      DR=R(JP)-R(JP+1)                                                  SPLIT    49
      R1=R2                                                             SPLIT    50
      R2=R(JP)                                                          SPLIT    51
```

```
      XM(JP)=DR*F2*(R1**IA+R2**IA+F3*R1*R2)/V(JP)                    SPLIT      52
      CF=CF/(XM(JP)+XM(JP+1))                                       SPLIT      53
      XM(JP)=XM(JP)*CF          Be sure mass is conserved exactly   SPLIT      54
      XM(JP+1)=XM(JP+1)*CF                                          SPLIT      55
   10 CONTINUE                                                      SPLIT      56
      RETURN                                                        SPLIT      57
      END                                                           SPLIT      58
```

SPLIT

Splits N cells starting at cell #J into two cells. All cell quantities are linearly interpolated and conservation of mass is explicitly required.

Local Variables

JJ = cell # being split.

JP = cell # to which the split is made.

JM = JJ - 1.

CF = (1) mass of cell being split, (2) ratio of computed mass to original mass.

DR = cell width.

Notes

Cells are divided in half and the new cell quantities are linear (in Lagrangian coordinates) interpolations of the old cell quantities. The cell masses are adjusted from the interpolation such that mass is conserved exactly.

```
      SUBROUTINE EPP(I,J)                                                    EPP        2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,              PARAM      2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                       PARAM      3
     +MXDUMP=30,MDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                         PARAM      4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                             PARAM      5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                              MCELL      2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)        MCELL      3
     +,W(MCL)                                                                MCELL      4
      LEVEL 2,R                                                              MCELL      5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM,      MCELL      6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                         MCELL      7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                       MCELL      8
      LEVEL 2,TIME                                                           MCELL      9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO      INIT       2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML),     INIT       3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)                 INIT       4
      COMMON/BRND/Z(ML),E(ML),VCJ(ML),DWDT(NDW,ML),PCJ(ML),PM(ML),ND(ML)     BRD        2
     +,MSFF                                                                  BRD        3
      IF(TMLT(I).LE.0.)GO TO 10                                              EPP        7
      TM=TMLT(I)+TMC(I)*(VO(I)-V(I))/VO(I)   Kennedy melt law                EPP        8
      IF(TM.GT.T(J))GO TO 10                                                 EPP        9
      SX(J)=0.                                                               EPP       10
      SZ(J)=0.                                                               EPP       11
      RETURN                                                                 EPP       12
   10 CONTINUE                                                               EPP       13
      GO TO (1,3,1),IALPH                                                    EPP       14
1     IF(P(J).LT.0.)GO TO 2  No correction for negative pressures            EPP       15
      IF(PLAP(I).LT.YO(I))GO TO 2  No correction if PLAP < 2/3 Y0            EPP       16
      X=P(J)/PLAP(I)                                                         EPP       17
      P(J)=P(J)-YO(I)*AMIN1(1.,X)   Correction to get on the hydrostat       EPP       18
2     IF(ABS(SX(J)).LE.YO(I))GO TO 4   On the yield surface?                 EPP       19
      SX(J)=SIGN(YO(I),SX(J))                                                EPP       20
4     P(J)=P(J)+SX(J)   Total stress in the x-direction                      EPP       21
      RETURN                                                                 EPP       22
3     CONTINUE                                                               EPP       23
      IF(P(J).LT.0.)GO TO 5                                                  EPP       24
      IF(PLAP(I).LT.YO(I))GO TO 5                                            EPP       25
      X=P(J)/PLAP(I)                                                         EPP       26
      P(J)=P(J)-YO(I)*AMIN1(1.,X)                                            EPP       27
    5 F=2*(SX(J)*(SX(J)+SZ(J))+SZ(J)*SZ(J))   Yield surface for α = 2 is     EPP       28
      TTY2=1.5*YO(I)*YO(I)                                  different        EPP       29
      IF(F.LT.TTY2)GO TO 4                                                   EPP       30
      FT=SQRT(TTY2/F)                                                        EPP       31
      SX(J)=FT*SX(J)   Sx and Sz are independent                             EPP       32
      SZ(J)=SZ(J)*FT                                                         EPP       33
      GO TO 4                                                                EPP       34
      RETURN                                                                 EPP       35
      END                                                                    EPP       36
```

EPP

An elastic — perfectly plastic model with the von Mises yield model and an optional correction term to put shock data fit equations of state on the hydrostat.

Local Variables

X = P/PLAP. See below for usage.

Notes

In the elastic region, consider the linear stress-strain relation (Hooke's Law),

$$\sigma_{ij} = 2\mu\varepsilon_{ij} + \lambda(\varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33}) \quad . \tag{1}$$

The hydrostat is given by $\varepsilon_{ii} = -\Delta V/3V$ for all i and

$$P_{\text{hydrostat}} = -\left(\frac{2\mu}{3} + \lambda\right)\frac{\Delta V}{V} \quad . \tag{2}$$

For one-dimensional compression we have $\varepsilon_{11} = -\Delta V/V$ with all other $\varepsilon_{ii} = 0$. This gives

$$P_{\text{Hugoniot}} = \sigma_{11} = -(2\mu + \lambda)\,\frac{\Delta V}{V} \tag{3}$$

and

$$\sigma_{22} = \sigma_{33} = -\lambda\frac{\Delta V}{V} \quad , \tag{4}$$

with

$$\sigma_{11} - \sigma_{22} = -2\mu\,\frac{\Delta V}{V} \quad . \tag{5}$$

The value determined experimentally is P_{Hugoniot} in single shock compression. For strains larger than at the yield point, $\sigma_{11} - \sigma_{22}$ is assumed to remain constant at Y_0, the yield stress. The difference between the Hugoniot stress and the hydrostat is

$$P_{Hug} - P_{hydro} = -\frac{4}{3}\mu\frac{\Delta V}{V} \tag{6}$$

in the elastic region. At the yield point, $-\Delta V^{Y} = Y_0 V/2\mu$ and $P^{Y}_{Hug} = ((2\mu+\lambda)/2\mu)Y_0$. The difference between P_{Hug} and P_{hydro} can then be written as

$$P_{Hug} - P_{hydro} = \frac{2}{3} Y_0 \frac{P_{Hug}}{P^{Y}_{Hug}} = -\frac{4}{3}\mu\frac{\Delta V}{V} \quad . \tag{7}$$

In a similar manner, we can write for strains larger than at the yield point,

$$P_{Hug} - P_{hydro} = \frac{2}{3} Y_0 \quad . \tag{8}$$

These last two formulas are found to be in satisfactory agreement with experiment for real materials in the region of interest. They are then used to calculate the hydrostat for equations of state fit to Hugoniot data. In the code P^{Y}_{Hug} is designated PLAP and is input data. For PLAP $< \frac{2}{3} Y_0$, it is assumed that the EOS pressure is the hydrostat.

Next we define the stress deviators by

$$S_i = \sigma_i - P \quad , \tag{9}$$

where

$$P = \frac{\sigma_1 + \sigma_2 + \sigma_3}{3} \tag{10}$$

and

$$\sigma_i = 2\mu\varepsilon_i + \lambda(\varepsilon_1 + \varepsilon_2 + \varepsilon_3) \quad , \tag{11}$$

which is Eq. (1) with a change of notation to take advantage of the fact that σ_{ij} is diagonal for the coordinate systems we are considering.

Substitution of Eq. (11) in Eqs. (9) and (10) gives

$$S_i = 2\mu(\varepsilon_i + \frac{\Delta V}{3V}) \quad , \tag{12}$$

with

$$P = -\left(\frac{2\mu}{3} + \lambda\right) \frac{\Delta V}{V} \quad , \tag{13}$$

where we have used

$$-\frac{\Delta V}{V} = \varepsilon_1 + \varepsilon_2 + \varepsilon_3 \quad . \tag{14}$$

The differential form of Eq. (12),

$$\dot{S}_i = 2\mu(\dot{\varepsilon}_i + \frac{\dot{V}}{3V}) \quad , \tag{15}$$

is used in the code to calculate the stress deviators.

The yield stress is calculated using the von Mises yield criteria. This model assumes that yielding occurs when the distortion energy is the same as the distortion energy at yield for simple tension (see, e.g., Mendelson, Plasticity: Theory and Application for further details). This criterion can be written as

$$\frac{1}{2}\left[(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2\right] = Y_0^2 \quad , \tag{16}$$

which can be rewritten in terms of the stress deviators to give

$$S_1^2 + S_2^2 + S_2^2 = \frac{2}{3} Y_0^2 \quad . \tag{17}$$

For $\alpha = 1$ and $\alpha = 3$, directions 2 and 3 are equivalent so we have

$$S_2 = S_3 = -\frac{1}{2} S_1 \quad , \tag{18}$$

which simplifies Eq. (17) to yield

$$S_1 = \frac{2}{3} Y_0 \quad . \tag{19}$$

Equation 15 need only be evaluated in the 1-direction, which is the x-direction for $\alpha = 1$ and the r-direction (still denoted x in the code) for $\alpha = 3$. The value for $\dot{\varepsilon}_1$ is obtained from

$$\dot{\varepsilon}_1 = - \frac{\partial U}{\partial R} \quad , \tag{20}$$

which is the same for all α.

For $\alpha = 2$, none of the directions are equivalent, so we have

$$S_2 = -S_1 - S_3 \quad , \tag{21}$$

which is substituted into Eq. (17) to give

$$f \equiv 2(S_1^2 + S_3^2 + S_1 S_3) = \frac{2}{3} Y_0^2 \quad . \tag{22}$$

The value for $\dot{\varepsilon}_1$ is again obtained from Eq. (20). However, the value for $\dot{\varepsilon}_3$ is zero because the 3-direction, which is the z-direction, does not have any motion in cylindrical geometry. When the yield condition, Eq. (22), is met, the stress deviators in the 1- and 3-directions are scaled to lie on the yield surface.

```
      SUBROUTINE DELT                                                    DELT      2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,          PARAM     2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                   PARAM     3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                     PARAM     4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                         PARAM     5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                          MCELL     2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)    MCELL     3
     +,W(MCL)                                                            MCELL     4
      LEVEL 2,R                                                          MCELL     5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM,  MCELL     6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                     MCELL     7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                   MCELL     8
      LEVEL 2,TIME                                                       MCELL     9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO  INIT      2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML),INIT      3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)             INIT      4
      COMMON/VOID/TNTX(ML2),JV(ML2),IV(ML2),NNV                          VD        2
      COMMON/MNMX/KMAX(ML2),KMIN(ML2),NMC                                MN        2
      COMMON/BRNS/A(ML),BR(ML),BA(ML),VBO(ML),VBSW(ML)                   BRN       2
      COMMON/EOSN/IEOS(ML),ME(ML)                                        EN        2
      COMMON/ES/IE(ML2),NME                                              ESM       2
      DATA IDV/0/                                                        DELT     11
      NMCE=IE(NMC)                                                       DELT     12
      IF(JMAX(NMC)-JMIN(NMC).LE.2.AND.NMC.GT.1)NMCE=IE(NMC-1)            DELT     13
      IF(DTO(NMCE).LE.DT)DTF=DTO(NMCE)                                   DELT     14
      IF(NDELT.EQ.1.OR.IBRN(NMC).EQ.3)RETURN                             DELT     15
      DTC=DTO(NMCE)                                                      DELT     16
      DLT=DTO(NMCE)                                                      DELT     17
      JI=0                                                               DELT     18
      DO 10 I=1,NMC                                                      DELT     19
      II=IE(I)                                                           DELT     20
      JMN=JMIN(I)                                                        DELT     21
      JMX=JMAX(I)                                                        DELT     22
      VM=V(JMN)                                                          DELT     23
      DRM=R(JMN)-R(JMN+1)                                                DELT     24
      DRV=DRM                                                            DELT     25
      JJ=JMN                                                             DELT     26
      JR=JMN                                                             DELT     27
      JMN=JMN+1                                                          DELT     28
      DO 11 J=JMN,JMX          Find the smallest ΔR in the region        DELT     29
      DR=R(J)-R(J+1)                                                     DELT     30
      IF(DR.GT.DRM)GO TO 12                                              DELT     31
      JR=J                                                               DELT     32
      DRM=DR                                                             DELT     33
   12 CONTINUE                                                           DELT     34
      IF(V(J).GE.VM)GO TO 11                                             DELT     35
      JJ=J                     Find the smallest V in the region         DELT     36
      VM=V(J)                                                            DELT     37
      DRV=DR                                                             DELT     38
   11 CONTINUE                                                           DELT     39
      DTC=DTCF(NMCE)*DRM/C(II,JR)   Δt for the smallest  R               DELT     40
      IF(DTC.LT.DLT)DLT=DTC    Is it smaller than DLT?                   DELT     41
      IF(JR.EQ.JJ)GO TO 10   Don't check the same cell twice             DELT     42
      DTC=DTCF(NMCE)*DRV/C(II,JJ)  Δt for the smallest V                 DELT     43
      IF(DTC.LT.DLT)DLT=DTC   Is it smaller than DLT?                    DELT     44
   10 CONTINUE                                                           DELT     45
      J=KMAX(NM)+1                                                       DELT     46
      IF(IA.EQ.0)GO TO 20          Check for last cell about to hit the origin DELT 47
      IF(R(J).LE.1.E-10)GO TO 20    (α = 2 or 3) and whether the time step is DELT 48
      IF(U(J).GE.0.)GO TO 20        small enough                         DELT     49
```

```
      DTV=-R(J)/U(J)                                                    DELT      50
      IF(DTV.GT.5*DT)GO TO 20                                           DELT      51
      DLTV=-.05*(R(J-1)-R(J))/U(J-1)                                    DELT      52
      IF(DLTV.GT.DLT)GO TO 20                                           DELT      53
      DT1=DLTV                                                          DELT      54
      IDV=101                                                           DELT      55
   20 CONTINUE                                                          DELT      56
      IF(NNV.LE.0) GO TO 40                                             DELT      57
      DO 30 I=1,NMC                                                     DELT      58
      IF(IV(I).NE.0) GO TO 30                                           DELT      59
      J=JV(I)                                                           DELT      60
      DRV=R(J)-R(J+1)                                                   DELT      61
      DU=U(J)-U(J+1)                                                    DELT      62
      IF(DU.GT.-0.01)GO TO 30                                           DELT      63
      DTV=-DRV/DU          Check for void about to collapse             DELT      64
      IF(DTV.GT.5*DT)GO TO 30                                           DELT      65
      DRM=R(J-1)-R(J)                                                   DELT      66
      DRP=R(J+1)-R(J+2)                                                 DELT      67
      DRT=AMIN1(DRP,DRM)                                                DELT      68
      DTV=0.05*DRT/ABS(DU)                                              DELT      69
      IF(DTV.GT.DLTV)GO TO 30                                           DELT      70
      IDV=101                                                           DELT      71
      DLTV=DTV                                                          DELT      72
      DT1=DLTV                                                          DELT      73
   30 CONTINUE                                                          DELT      74
   40 CONTINUE                                                          DELT      75
      IDV=IDV-1                                                         DELT      76
      IF(DLT.LT.DTO(NMCE))DTF=DLT                                       DELT      77
      IF(IDV.GE.1)DTF=DT1      Pick the smallest time step              DELT      78
      IF(DLT.LT.DTF)DTF=DLT                                             DELT      79
      DTR=DTF/DT                                                        DELT      80
      IF(DTR.LT.0.9.OR.DTR.GT.1.2)DT=DTF   Don't make small changes in Δt DELT      81
      RETURN                                                            DELT      82
      END                                                               DELT      83
```

DELT

Calculates the time step to be used. The time step may be input data or may be evaluated from several criteria in order to keep the problem numerically stable.

Local Variables

IDV = index used to count the number of time steps to use the void collapse time step.

NMCE = the region from which the maximum allowed time step is obtained.

DTC = Δt calculated from the sound speed.

DLT = variable used to keep track of the lowest calculated Δt.

II = IE(I) = original region #.

JMN = JMIN(I).

JMX = JMAX(I).

VM = variable used to find the smallest volume in the region.

DRM = variable used to find the smallest Δr in the region.

JJ = cell # of cell with V = VM.

JR = cell # of cell with Δr = DRM.

J = last cell # in the problem/void cell #.

DTV = time step required for cell with Δr = DRT to collapse 5% when void collapses - also, approximate time required for the inner surface of the problem to reach the origin.

DLTV = time step required to collapse the last cell 5% when it hits the origin.

DT1 = DLTV when small enough to be needed = collapse time step.

DRV = width of void.

DU = relative velocity at which a void is closing.

DTV = approximate time required for a void to close.

DRM = Δr for cell that is outside bound of a void.

DRP = Δr for a cell that is inside bound of a void.

DRT = smaller of the two.

DTR = ratio of computed time step to the current time step.

Notes

Several methods are used to compute the time step. For a sharp shock burn, Δt is fixed in SSB (q.v.) and is not changed by DELT. Each region can be assigned a maximum time step, DTO, which is in effect when that region is the last active region. For NDELT = 1 in the INP namelist, Δt is set to DTO for the last active region. The time step can also be calculated from a constant times the time it takes a sound wave to cross a cell at the local sound speed. That is, $\Delta t = a(\Delta r/c)$, where a is a constant (DTCF in the code with default value of 1/2), Δr is the cell width, and c is the sound speed in that cell. This check is made for the densest cell and the cell with the smallest width for each material. (See Chap. 12 of Richtmyer and Morton, Differential Methods for Initial-Value Problems, 2nd Ed., for a discussion of the stability criteria for the difference equations.)

In converging geometry, for the inside surface about to collapse at the origin, the time step is temporarily (100 cycles) required to be no greater than 1/20 of the time required for the outside of the innermost cell to reach the origin at its current velocity. The same criteria is used for collapsing voids, except that the relative velocity of the two surfaces is used along with the smaller of the two cell widths for the cells touching the void.

```
      FUNCTION C(I,J)                                                    C          2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,          PARAM      2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                   PARAM      3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                     PARAM      4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                         PARAM      5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                          MCELL      2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)    MCELL      3
     +,W(MCL)                                                            MCELL      4
      LEVEL 2,R                                                          MCELL      5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM,  MCELL      6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                     MCELL      7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                   MCELL      8
      LEVEL 2,TIME                                                       MCELL      9
      COMMON/EOSN/IEOS(ML),ME(ML)                                        EN         2
      IS=IEOS(I)                                                         C          6
      VJ=V(J)                                                            C          7
      PJ=P(J)                                                            C          8
      XIJ=XI(J)                                                          C          9
      GO TO (1,2,3,4),IS    Pick sound speed subroutine according to EOS type  C     10
    1 CALL CUSUP(VJ,PJ,CC,I)                                             C         11
      C=CC                                                               C         12
      RETURN                                                             C         13
    2 CALL CBLDUP(I,J,CC)                                                C         14
      C=CC                                                               C         15
      RETURN                                                             C         16
    3 CALL CPOLY(VJ,PJ,XIJ,CC,I)                                         C         17
      C=CC                                                               C         18
      RETURN                                                             C         19
    4 CALL CSES(VJ,XIJ,CC,I,J)                                           C         20
      C=CC                                                               C         21
      RETURN                                                             C         22
      END                                                                C         23
```

C

Switching function subroutine to pick the appropriate sound speed subroutine.

Local Variables

IS = IEOS(I) = equation-of-state type.

VJ = V(J).

PJ = P(J).

XIJ = XI(J).

CC = sound speed.

C = sound speed.

```
      SUBROUTINE CUSUP(VC,PC,C,I)                                       CUSUP      2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM      2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM      3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM      4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                        PARAM      5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                         MCELL      2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)   MCELL      3
     +,W(MCL)                                                           MCELL      4
      LEVEL 2,R                                                         MCELL      5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM, MCELL      6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                    MCELL      7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                  MCELL      8
      LEVEL 2,TIME                                                      MCELL      9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO  INIT       2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT       3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)            INIT       4
      COMMON/USUPC/C1(ML),S1(ML),C2(ML),S2(ML),SWV(ML),VMN(ML),         US         2
     +GAMMA(ML),ALP(ML)                                                 US         3
      COMMON/BRNS/A(ML),BR(ML),BA(ML),VBO(ML),VBSW(ML)                  BRN        2
      IF(IBRN(I).NE.0)GO TO 40                                          CUSUP      8
      IF(VC.GT.SWV(I)) GO TO 11                                         CUSUP      9
12    C=C2(I)                                                           CUSUP     10
      S=S2(I)                                                           CUSUP     11
      GO TO 20                                                          CUSUP     12
11    C=C1(I)                                                           CUSUP     13
      S=S1(I)                                                           CUSUP     14
20    ETA=(VO(I)-VC)/VO(I)                                              CUSUP     15
      IF(PC.LE.0.) GO TO 30                                             CUSUP     16
      VV=VC/VO(I)                                                       CUSUP     17
      HP=(C/(1-S*ETA))**2*ETA/VO(I)                                     CUSUP     18
      CSQ=(VV*C)**2*(1+S*ETA)*(1-GAMMA(I)*ETA/(2*VV))                   CUSUP     19
     +/(1-S*ETA)**3+GAMMA(I)*VO(I)*HP/2+VC*(PC-HP)*(GAMMA(I)+1)         CUSUP     20
      IF(CSQ .LE. 0) GO TO 30                                           CUSUP     21
      C=SQRT(CSQ)                                                       CUSUP     22
30    CONTINUE                                                          CUSUP     23
      RETURN                                                            CUSUP     24
40    C=1.                                                              CUSUP     25
      RETURN                                                            CUSUP     26
      END                                                               CUSUP     27
```

Pick appropriate USUP constants

If in tension, use C from USUP constants

Hugoniot pressure

C^2

If $C^2 < 0$, use C from USUP constants

Used for HE's

CUSUP(VC,PC,C,I)

Calculates the sound speed for a USUP EOS with constant Grüneisen γ.

Local Variables

VC = specific volume, V, for which C is to be calculated (subroutine argument).

PC = pressure, P, for which C is to be calculated (subroutine argument).

C = sound speed = output of subroutine (subroutine argument).

I = initial region number from which to get EOS constants (subroutine argument).

S = S in USUP fit $U_S = C + SU_P$

ETA = $\eta = \dfrac{V_0 - V}{V_0}$.

VV = $\dfrac{V}{V_0} = 1 - \eta$.

HP = Hugoniot pressure at specific volume V.

CSQ = C^2.

Notes

The sound velocity C is given by

$$C^2 = \left(\frac{\partial P}{\partial \rho}\right)_S = -V^2\left(\frac{\partial P}{\partial V}\right)_S \quad , \tag{1}$$

which can be rewritten as

$$C^2 = -V^2\left[\left(\frac{\partial P}{\partial I}\right)_V\left(\frac{\partial I}{\partial V}\right)_S + \left(\frac{\partial P}{\partial V}\right)_I\left(\frac{\partial V}{\partial V}\right)_S\right] = V^2\left[P\left(\frac{\partial P}{\partial I}\right)_V - \left(\frac{\partial P}{\partial V}\right)_I\right] . \tag{2}$$

The Grüneisen EOS is given by

$$P = P_H + \frac{\gamma}{V}(I - I_H) \quad , \tag{3}$$

where

$$P_H = \rho_0 c_0^2 \eta/(1 - S\eta)^2 \quad , \tag{4}$$

$$I_H = \frac{P_H \eta V_0}{2} \quad , \tag{5}$$

with P_0 and I_0 ignored, and

$$\eta = \frac{V_0 - V}{V_0} \quad . \tag{6}$$

Since P_H is a function of volume only, the first term in Eq. (2) is readily evaluated using Eq. (3) to give

$$P\left(\frac{\partial P}{\partial I}\right)_V = P \frac{\gamma}{V} \quad , \tag{7}$$

where γ is assumed to be constant.

The second term in Eq. (2) is more readily evaluated if we rewrite Eq. (3) in the form

$$P = P_H\left(1 - \frac{\gamma \eta V_0}{2V}\right) + \frac{I\gamma}{V} \quad . \tag{8}$$

We then have

$$\left(\frac{\partial P}{\partial V}\right)_I = \frac{\partial P_H}{\partial V}\left(1 - \frac{\eta \gamma V_0}{2V}\right) + \frac{P_H \gamma V_0}{2V^2} - \frac{I\gamma}{V^2} \quad , \tag{9}$$

where

$$\frac{\partial P_H}{\partial V} = \frac{\partial P_H}{\partial \eta}\frac{\partial \eta}{\partial V} = -\left(\frac{C_0}{V_0}\right)^2\left(\frac{1 + S\eta}{(1 - S\eta)^3}\right) \tag{10}$$

and I can be written from Eq. (8) as

$$I = \frac{V}{\gamma}\left[P - P_H\left(1 - \frac{\eta\gamma V_0}{V}\right)\right] \quad . \tag{11}$$

Substitution of Eqs. (6), (7), (9), (10), and (11) in Eq. (2) yields

$$C^2 = V^2\left\{\frac{P\gamma}{V} - \frac{\partial P_H}{\partial V}\left(1 - \frac{\eta\gamma V_0}{2V}\right) - P_H\frac{\gamma V_0}{2V^2} + \frac{1}{V}\left[P - P_H\left(1 - \frac{\eta\gamma V_0}{V}\right)\right]\right\}$$

$$= \left(\frac{C_0 V}{V_0}\right)^2 \frac{(1 + S\eta)}{(1 - S\eta)^3}\left(1 - \frac{\eta\gamma V_0}{2V}\right) + (P - P_H)(\gamma + 1) + P_H\frac{\gamma V_0}{2} \quad . \tag{12}$$

If $C^2 < 0$ or $P < 0$, then C is set to C_0, the sound speed in the uncompressed solid. The value of C_0 and S that is used is allowed to be one of two sets of values depending on the volume. See USUP for more details.

```
      SUBROUTINE CALDUP(I,J,CC)                                          CBLDUP     2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,          PARAM      2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                   PARAM      3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                     PARAM      4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                         PARAM      5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                          MCELL      2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)    MCELL      3
     +,W(MCL)                                                            MCELL      4
      LEVEL 2,R                                                          MCELL      5
      COMMON/DVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM,  MCELL      6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                     MCELL      7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                   MCELL      8
      LEVEL 2,TIME                                                       MCELL      9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO  INIT       2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT       3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)             INIT       4
      COMMON/BUX/BUA,BUB,BUMAX,BUDV(ML)                                  BUP        2
     +,BUR,BUD                                                           BUP        3
      COMMON/ES/IE(ML2),NME                                              ESM        2
      JMN=JMIN(I)                                                        CBLDUP     8
      JMX=JMAX(I)                                                        CBLDUP     9
      II=IE(I)                                                           CBLDUP    10
      IF(W(J).GT.0.99)GO TO 10                                           CBLDUP    11
      IF(W(JMX).GT.0.99.OR.W(JMN).GT.0.99)GO TO 10  If still burning, use D CBLDUP 12
      B=(T(J)-.66)/(T(J)*(T(J)-2.32))   β                                CBLDUP    13
      B=(B+1)/B                                                          CBLDUP    14
      VV=T(J)*VO(II)/(V(J)*(T(J)+1))                                     CBLDUP    15
      PI=(ROW(II)*BUDV(II)*VV**T(J))/(T(J)+1)   Reference pressure       CBLDUP    16
      CC=SQRT((B*(P(J)/(1-W(J))-PI)+T(J)*PI)*V(J))  C                    CBLDUP    17
      IF(CC.LT.0.2)CC=0.2   Lower limit on C                             CBLDUP    18
      RETURN                                                             CBLDUP    19
   10 CONTINUE                                                           CBLDUP    20
      CC=SQRT(BUDV(II))   Use the detonation velocity for C              CBLDUP    21
      RETURN                                                             CBLDUP    22
      END                                                                CBLDUP    23
```

CBLDUP

Calculates the sound speed for a buildup EOS in cell J.

Local Variables

II = IE(I) = original region #.

JMN = JMIN(I).

JMX = JMAX(I).

$B = \frac{\beta + 1}{\beta}$.

VV = V_{CJ}/V.

PI = P_i = reference pressure.

CC = sound speed.

Notes

The buildup EOS (see BLDUP for details) is given by

$$P = \left[\frac{1}{\beta V}\left(I - K - \frac{P_i V}{\gamma - 1}\right) + P_i\right](1 - W) \quad , \tag{1}$$

where P_i is the reference pressure,

$$P_i = P_{CJ} * \left(\frac{V_{CJ}}{V}\right)^{\gamma} = \frac{\rho_0 D^2}{\gamma + 1}\left(\frac{\gamma V_0}{(\gamma + 1)V}\right)^{\gamma} \quad , \tag{2}$$

and β is given by

$$\beta = \frac{\gamma - 0.66}{\gamma(\gamma - 2.32)} \quad , \tag{3}$$

and K is a constant for fixed γ (note γ is stored in T(J)).

The square of the sound speed, C^2, is (see CUSUP)

$$C^2 = V^2\left[P\left(\frac{\partial P}{\partial I}\right)_V - \left(\frac{\partial P}{\partial V}\right)_I\right] \quad . \tag{4}$$

Combining Eq. (1) and Eq. (4) we find

$$c^2 = \left(\frac{\beta + 1}{\beta^2}\right)\left(I - K - \frac{P_i V}{\gamma - 1}\right) + \gamma P_i V = \left(\frac{\beta + 1}{\beta}\right)\left(\frac{P}{1 - W} - P_i\right)V + \gamma P_i V \quad . \qquad (5)$$

Now, if W(J) is too near 1, there is the possibility of numerical problems. Also, the calculated sound speed will be small. Since the buildup burn model is designed for prompt detonation, the detonation velocity is used for the sound speed when W(J) > 0.99. It is also used if either the innermost or outermost cell of the region has W > 0.99. We have arbitrarily set the lower limit of the sound speed at 0.2 cm/μs.

```
      SUBROUTINE CPOLY(VC,PC,XC,C,I)                                    CPOLY      2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM      2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM      3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM      4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                        PARAM      5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                         MCELL      2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)   MCELL      3
     +,W(MCL)                                                           MCELL      4
      LEVEL 2,R                                                         MCELL      5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM, MCELL      6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                    MCELL      7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                  MCELL      8
      LEVEL 2,TIME                                                      MCELL      9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO  INIT       2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT       3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)            INIT       4
      COMMON/POLYC/CF(NCF,ML),PS(ML)                                    PLC        2
      VP=VO(I)/VC                                                       CPOLY      7
      VV=VP-1.   η                                                      CPOLY      8
      VP=-VP/VC    η'                                                   CPOLY      9
      A=VV*(CF(1,I)+CF(2,I)*ABS(VV))   A                                CPOLY     10
      B=CF(3,I)+VV*(CF(4,I)+VV*CF(5,I))  B                              CPOLY     11
      C=CF(6,I)+CF(7,I)*VV   C                                          CPOLY     12
      AP=VP*(CF(1,I)+2*CF(2,I)*ABS(VV))   A'                            CPOLY     13
      BP=VP*(CF(4,I)+2*CF(5,I)*ABS(VV))   B'                            CPOLY     14
      CP=VP*CF(7,I)  C'                                                 CPOLY     15
      XIC=XC*ROW(I)   ε                                                 CPOLY     16
      DPDV=((PC*ROW(I)*(B+2*XIC*C)-(A+XIC*(B+XIC*C))/(XIC+CF(8,I)))     CPOLY     17
     +-(AP+XIC*(BP+XIC*CP)))/(XIC+CF(8,I))                              CPOLY     18
      IF(DPDV.LT.0.)DPDV=CF(1,I)/CF(8,I)  -(∂P/∂V)s                     CPOLY     19
      C=VC*SQRT(DPDV)   C                                               CPOLY     20
      RETURN                                                            CPOLY     21
      END                                                               CPOLY     22
```

CPOLY(VC,PC,XC,C,I)

Calculates the sound speed at specific volume VC, pressure PC, and specific internal energy XC for the eight-parameter fit EOS in subroutine POLY.

Local Variables

$VP = \frac{\partial \eta}{\partial V}$.

$VV = \frac{V_0 - V}{V} = \eta$.

A,B,C = see notes.

$AP = \frac{\partial A}{\partial V}$.

$BP = \frac{\partial B}{\partial V}$.

$CP = \frac{\partial C}{\partial V}$.

$XIC = \rho_0 I = \varepsilon$.

$DPDV = \left(\frac{\partial P}{\partial V}\right)_S$.

C = sound speed, $C^2 = -V^2\left(\frac{\partial P}{\partial V}\right)_S$.

Notes

As shown in CUSUP, the square of the sound velocity can be written

$$C^2 = -V^2\left(\frac{\partial P}{\partial V}\right)_S = V^2\left[P\left(\frac{\partial P}{\partial I}\right)_V - \left(\frac{\partial P}{\partial V}\right)_I\right] . \tag{1}$$

The POLY EOS is

$$P = \frac{A + B\varepsilon + C\varepsilon^2}{\varepsilon + C_8} , \tag{2}$$

where

$$A = \eta C_1 + |\eta|\eta C_2 , \tag{3}$$

$$B = C_3 + \eta C_4 + \eta^2 C_5 , \tag{4}$$

and

$$C = C_6 + \eta C_7 \quad , \tag{5}$$

with

$$\eta = \frac{V_0 - V}{V} \tag{6}$$

and

$$\varepsilon = \rho_0 I \quad . \tag{7}$$

The bracket is readily evaluated to give

$$-\left(\frac{\partial P}{\partial V}\right)_S = P\rho_0\left(\frac{B + 2\varepsilon C}{\varepsilon + C_8} - \frac{A + B\varepsilon + C\varepsilon^2}{(\varepsilon + C_8)^2}\right) - \frac{A' + \varepsilon B' + \varepsilon^2 C'}{\varepsilon + C_8} \quad , \tag{8}$$

where

$$A' = \frac{\partial A}{\partial V} = \frac{\partial A}{\partial \eta}\frac{\partial \eta}{\partial V} = (C_1 + 2C_2|\eta|)\eta' \quad , \tag{9}$$

$$B' = \frac{\partial B}{\partial \eta}\frac{\partial \eta}{\partial V} = (C_4 + \eta C_5)\eta' \tag{10}$$

$$C' = \frac{\partial C}{\partial \eta}\eta' = C_7\eta' \quad , \tag{11}$$

with

$$\eta' = \frac{\partial \eta}{\partial V} = -\frac{V_0}{V^2} \quad . \tag{12}$$

A check is made whether $-\left(\frac{\partial P}{\partial V}\right)_S$ is positive. If it is not, the $\eta = 0$, $I = 0$ value (initial conditions) is used, which is

$$-\left(\frac{\partial P}{\partial V}\right)_S^0 = -\frac{A'(\eta=0)}{C_8} = \frac{C_1}{C_8 V_0} \quad . \tag{13}$$

The sound velocity is then

$$C = V\sqrt{-\left(\frac{\partial P}{\partial V}\right)_S} \quad . \tag{14}$$

```
      SUBROUTINE CSES(VJ,XIJ,CC,I,J)                                    CSES       2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM      2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM      3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM      4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                        PARAM      5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                         MCELL      2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)   MCELL      3
     +,W(MCL)                                                           MCELL      4
      LEVEL 2,R                                                         MCELL      5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM, MCELL      6
     +IALPH,NDELT,LAPEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                    MCELL      7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                  MCELL      8
      LEVEL 2,TIME                                                      MCELL      9
      COMMON/ES/IE(ML2),NME                                             ESM        2
      COMMON/SESIN/II,IDT,RPT4,XIPT4,IBR,IFL                            CSES       7
      COMMON/SESOUT/PPT4(3),TPT4(3)                                     CSES       8
      CC=.5   Default value                                             CSES       9
      IBR=1   Output PPT4 only                                          CSES      10
      IDT=1                                                             CSES      11
      II=IE(I)                  ]                                       CSES      12
      XIPT4=XIJ                 ]  Set up input                         CSES      13
      RPT4=1./VJ                ]                                       CSES      14
      IFL=MOD(IFLAG(J),64)      ]                                       CSES      15
      CALL T4EOSA   Call SESAME                                         CSES      16
      C2=VJ*VJ*PPT4(1)*PPT4(3)+PPT4(2)   C^2                            CSES      17
      IF(C2.GT.0.)CC=SQRT(C2)   C                                       CSES      18
      RETURN                                                            CSES      20
      END                                                               CSES      21
```

CSES

Calculates the sound speed for a Sesame EOS.

Local Variables

CC = sound speed = C.

C2 = C^2.

Notes

The output of the Sesame EOS call in PPT4 is

$$\begin{aligned} \text{PPT4(1)} &= P \quad , \\ \text{PPT4(2)} &= \left(\frac{\partial P}{\partial \rho}\right)_I \quad , \\ \text{PPT4(3)} &= \left(\frac{\partial P}{\partial I}\right)_\rho \quad . \end{aligned} \tag{1}$$

The sound speed is given by

$$C^2 = V^2\left[P\left(\frac{\partial P}{\partial I}\right)_V - \left(\frac{\partial P}{\partial V}\right)_I\right] = V^2 P\left(\frac{\partial P}{\partial I}\right)_\rho + \left(\frac{\partial P}{\partial \rho}\right)_I \quad , \tag{2}$$

which in terms of the PPT4 array is

$$C^2 = V^2 * \text{PPT4(1)} * \text{PPT4(3)} + \text{PPT4(2)} \quad . \tag{3}$$

If the calculated C^2 is negative, then the default value of C = 1/2 is used.

```
      SUBROUTINE RLEOS(I)                                                RLEOS     2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,          PARAM     2
     +NUMV=10,MOL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                   PARAM     3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                     PARAM     4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                         PARAM     5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                          MCELL     2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)    MCELL     3
     +,W(MCL)                                                            MCELL     4
      LEVEL 2,R                                                          MCELL     5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM,  MCELL     6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TO(ML),IJK                     MCELL     7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                   MCELL     8
      LEVEL 2,TIME                                                       MCELL     9
      COMMON/VOID/INTX(ML2),JV(ML2),IV(ML2),NNV                          VD        2
      COMMON/RLC/RC(ML),RP(ML),RLV(ML),PH1,DV1,DV2                       RLC       2
      JP=JV(I)+1                                                         RLEOS     7
      IF(V(JP-2).LT.RLV(I).OR.V(JP).LT.RLV(I+1))GO TO 10                 RLEOS     8
      JM=JP-2                                                            RLEOS     9
      Q(JP)=0.                                                           RLEOS    10
      Q(JM)=0.                                                           RLEOS    11
      P(JP)=V(JP)*RC(I+1)+RP(I+1)]   Rayleigh line EOS                   RLEOS    12
      P(JM)=V(JM)*RC(I)+RP(I)       ]                                    RLEOS    13
      RETURN                                                             RLEOS    14
   10 CONTINUE                                                           RLEOS    15
      IV(I)=1   Go back to normal EOS                                    RLEOS    16
      RETURN                                                             RLEOS    17
      END                                                                RLEOS    18
```

RLEOS(I)

The Rayleigh line in P-V space is used as an equation of state for the initial compression of the two cells touching an interface that has just become a closed void when the relative velocity of the two surfaces was large.

Local Variables

JP = JV(I) + 1 = cell # of inside cell touching the interface.

JM = JP - 2 = cell # of outside cell touching the interface.

Notes

The Rayleigh line is a straight line in P-V space that passes through the initial state (P_0,V_0) and the final state (P_f,V_f) for a shock. That is

$$P = P_0 + (P_f - P_0)\left(\frac{V_0 - V}{V_0 - V_f}\right) \quad . \tag{1}$$

The change in energy across the shock front using the Rayleigh line EOS is

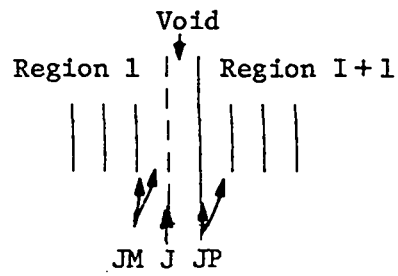
$$\Delta I = -\int_{V_0}^{V_f} PdV = P_0(V_0 - V_f) + \frac{(P_f - P_0)(V_0 - V_f)}{2} = \frac{(P_f + P_0)(V_0 - V_f)}{2} \quad , \tag{2}$$

which is equal to the energy change from the jump conditions. That is, without artificial viscosity, energy is conserved across the shock front using the Rayleigh line EOS. P_f and V_f are determined in RL using the jump conditions and equations of state for the two materials that collide. The RLEOS is used until one of the materials reaches a preset specific volume. RLV(I), at which time a flag is set to switch back to the normal EOS with artificial viscosity. Since the materials may be different, V_f can be different and the RLEOS would then be different. By the time the RLEOS is no longer used, the artificial viscosity is no longer so large that excessive energy is dumped in the cell before the difference equations have time to respond.

```
      SUBROUTINE RL(I)                                                  RL        2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM     2
     +NUMV=10,MOL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM     3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM     4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                        PARAM     5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                         MCELL     2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)   MCELL     3
     +,W(MCL)                                                           MCELL     4
      LEVEL 2,R                                                         MCELL     5
      COMMON/OVL/NDE,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM, MCELL     6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                    MCELL     7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                  MCELL     8
      LEVEL 2,TIME                                                      MCELL     9
      COMMON/RLC/RC(ML),RP(ML),RLV(ML),PH1,DV1,DV2                      RLC       2
      COMMON/VOID/INTX(ML2),JV(ML2),IV(ML2),NNV                         VD        2
      JP=JV(I)+1                                                        RL        7
      J=JP-1                                                            RL        8
      JM=JP-2                                                           RL        9
      DU=U(J)-U(JP)                                                     RL       10
      UV2=U(J)-DU/2      Initial guesses for interface velocity         RL       11
      GB=G(UV2,I)                                                       RL       12
      UV3=U(J)-DU*.45                                                   RL       13
      IC=0                                                              RL       14
   10 CONTINUE                                                          RL       15
      IC=IC+1                                                           RL       16
      UV1=UV2                                                           RL       17
      UV2=UV3                                                           RL       18
      IF(IC.GT.100)GO TO 11                                             RL       19
      GA=GB                                                             RL       20
      GB=G(UV3,I)        Iterate to find the velocity                   RL       21
      UV3=(GB*UV1-GA*UV2)/(GB-GA)   at which Hugoniot pressures         RL       22
      IF(UV3.LT.U(J).OR.UV3.GT.U(JP))GO TO 12   match                   RL       23
      IF(ABS((UV3-UV2)/UV3).GT.0.001)GO TO 10                           RL       24
      RC(I)=(P(JM)-PH1)/DV1                                             RL       25
      RC(I+1)=(P(JP)-PH1)/DV2                                           RL       26
      RP(I)=P(JM)-RC(I)*V(JM)                                           RL       27
      RP(I+1)=P(JP)-RC(I+1)*V(JP)                                       RL       28
      DR=R(J)-R(JP)                                                     RL       29
      A=(UV3-U(JP))/(U(J)-U(JP))                                        RL       30
      RV=A*R(J)+(1-A)*R(JP)   Set the Rayleigh line EOS parameters      RL       31
      U(J)=UV3                 and the interface velocity               RL       32
      U(JP)=U(J)                                                        RL       33
      R(J)=RV                                                           RL       34
      R(JP)=RV                                                          RL       35
      RLV(I)=V(JM)-0.9*DV1                                              RL       36
      RLV(I+1)=V(JP)-0.9*DV2                                            RL       37
      RETURN                                                            RL       38
   12 CONTINUE                                                          RL       39
      UV3=U(JP)-DU*.01                                                  RL       40
      UV2=U(J)+DU*.01    Fixup attempt if the iteration                 RL       41
      GB=G(UV2,I)         gets out of range                             RL       42
      GO TO 10                                                          RL       43
   11 CONTINUE                                                          RL       44
      PRINT 1,TIME,I,J                                                  RL       45
    1 FORMAT(18H RL ERROR AT TIME=,E13.4,4H I=,I3,4H J=,I4)             RL       46
      DR=R(J)-R(JP)                                                     RL       47
      R(J)=R(J)+U(J)*DR/DU   Iteration failed:                          RL       48
      R(JP)=R(J)              try the low-velocity method               RL       49
      U(J)=(U(J)+U(JP))/2                                               RL       50
      U(JP)=U(J)                                                        RL       51
      IV(I)=1                                                           RL       52
      RETURN                                                            RL       53
      END                                                               RL       54
```

RL(I)

Calculates parameters for the Rayleigh line EOS. This primarily consists of iteration to find the interface velocity which sends shock waves into both materials with the same final pressure.



Local Variables

JM,J,JP - see illustration.

After the collision, R(J) = R(JP) is the interface, U(J) = U(JP), and the void is closed.

DU = relative velocity of the two free surfaces.

UV1,UV2,UV3 = U_{i-2}, U_{i-1}, U_i. See notes.

GA,GB = g_i, g_{i+1}. See notes.

IC = count of # of iterations (only 100 are allowed).

DR = cell width.

RV = position of the interface after collision.

DTV = time the void has actually been closed.

Notes

The jump conditions (see USUP) can be combined to give the equations

$$I - I_0 = \frac{(P + P_0)(V_0 - V)}{2} \tag{1}$$

and

$$U_P = \sqrt{(P - P_0)(V_0 - V)} \quad , \tag{2}$$

where the subscript indicates initial quantities in the unshocked material and U_P is the particle velocity of the shocked material relative to the particle velocity of the unshocked material. Combining Eqs. (1) and (2), we have

$$I - I_0 = \frac{U_P^2}{2} + P_0(V_0 - V) \quad . \tag{3}$$

Now the shocks we are considering are from the collision of two free surfaces. At the free surface $P_0 = 0$, but P_0 can be nonzero at the center of a cell touching the collision interface. However, P_0 will be much less than P for the high-velocity collisions we are considering and will be set to zero in Eq. (3).

For the collision we are considering, the interface particle velocity, U, is the same for both materials. (We will designate the region outside the interface by superscript 1 and the inside region by 2.) By our choice of coordinates we will have the relation

$$U_0^{(2)} > U > U_0^{(1)} \quad , \tag{4}$$

where $U_0^{(1)}$ and $U_0^{(2)}$ are the free-surface velocities of regions 1 and 2 just before the collision. The corresponding particle velocities to be used with the jump conditions are

$$U_P^{(1)} = U - U_0^{(1)} \tag{5}$$

and

$$U_P^{(2)} = U_0^{(2)} - U \quad . \tag{6}$$

What we need to find is a value of U such that the Hugoniot pressure is the same on both sides of the interface. For a given value of U, we have a fixed value of I for each region from Eqs. (3), (5), and (6) (with $P_0 = 0$). Given I, V can be varied until a point on the Hugoniot (using Eq. (1) and the EOS) is found. We then define a function g(U)to be the difference in Hugoniot pressures for regions 1 and 2 when the interface velocity is U. The zero of g(U) is found using the secant method,

$$U_{i+1} = U_i - \frac{(U_i - U_{i-1})}{(g_i - g_{i-1})} g_i = \frac{U_{i-1}g_i - U_i g_{i-1}}{g_i - g_{i-1}} \quad . \tag{7}$$

Two initial values are set as

$$U_0 = U_0^{(1)} + \frac{1}{2}\left(U_0^{(2)} - U_0^{(1)}\right) \tag{8}$$

and

$$U_1 = U_0^{(1)} + .45\left(U_0^{(2)} - U_0^{(1)}\right) \quad , \tag{9}$$

where U_0 is the correct value if the two materials are the same and in the same state. If the iteration goes out of the range in Eq. (4), then new initial values

$$U_0 = U_0^{(1)} \tag{10}$$

and

$$U_1 = U_0^{(2)} \tag{11}$$

are tried. The iteration is allowed to proceed for 100 steps. If a solution has not been found, then an error message is printed and the low-velocity collision procedure is used.

When a solution for U is found, the parameters R_C and R_P for RLEOS are set. The Rayleigh line EOS can be written as

$$P = P_0 + (P_f - P_0)\frac{V_0 - V}{V_0 - V_f} = VR_C + R_P \quad , \tag{12}$$

where

$$R_C = \frac{P_0 - P_f}{V_0 - V_f} \tag{13}$$

and

$$R_P = P_0 + \frac{(P_f - P_0)V_0}{V_0 - V_f} = P_0 - R_C V_0 \quad . \tag{14}$$

A third parameter, R_ℓ, is the volume at which a flag is set in RLEOS to switch back to the normal EOS plus viscosity. It is given by

$$R_\ell = V_0 - 0.9(V_0 - V_f) \quad . \tag{15}$$

The interface velocity, U(J) = U(JP), is set to the solution value for U. The position of the interface, R(J) = R(JP), is found by a linear extrapolation back to the point of collision followed by uniform motion at velocity U.

```
 FUNCTION G(UV,I)                                                          G          2
 PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,                 PARAM      2
+NUMV=10,MOL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                          PARAM      3
+MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                           PARAM      4
+,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                               PARAM      5
 COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                                MCELL      2
+P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)          MCELL      3
+,W(MCL)                                                                  MCELL      4
 LEVEL 2,R                                                                MCELL      5
 COMMON/DVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM,         MCELL      6
+IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                           MCELL      7
 COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                         MCELL      8
 LEVEL 2,TIME                                                             MCELL      9
 COMMON/RLC/RC(ML),RP(ML),RLV(ML),PH1,DV1,DV2                             RLC        2
 COMMON/VOID/INTX(ML2),JV(ML2),IV(ML2),NNV                                VD         2
 COMMON/EOSN/IEOS(ML),ME(ML)                                              EN         2
 J=JV(I)                                                                  G          8
 JP=J+1                                                                   G          9
 JM=J-1    Given the interface velocity, calculate:                       G         10
 XI1=0.5*(UV-U(J))**2+XI(JM)    Internal energies                         G         11
 XI2=0.5*(U(JP)-UV)**2+XI(JP)                                             G         12
 PH1=PH(XI1,I,JM)                                                         G         13
 IP=I+1                                                                   G         14
 PH2=PH(XI2,IP,JP)              Hugoniot pressures                        G         15
 DV1=2*XI1/PH1                                                            G         16
 DV2=2*XI2/PH2                  Volume changes                            G         17
 G=PH1-PH2                      Pressure difference (= iteration function) G        18
 RETURN                                                                   G         19
 END                                                                      G         20
```

G(UV,I)

Given a value for the interface particle velocity, UV, the difference in the corresponding Hugoniot pressures of the two bounding cells is calculated.

Local Variables

JM,J,JP - see RL.

XI1 = specific internal energy for region 1. (See RL for definition of regions.)

XI2 - specific internal energy for region 2.

IP = I+1 = region # for region 2. (I = region # for region 1.)

PH2 = Hugoniot pressure for region 2.

Notes

We will reproduce here Eqs. (3), (5), and (6) from RL (with P_0 set to zero).

$$I = I_0 + \frac{U_P^2}{2} \quad . \tag{1}$$

$$U_P^{(1)} = U - U_0^{(1)} \quad . \tag{2}$$

$$U_P^{(2)} = U_0^{(2)} - U \quad . \tag{3}$$

These equations give the specific internal energy on the Hugoniot $I_H^{(1)}$ and $I_H^{(2)}$ for regions 1 and 2 consistent with an interface velocity U. The Hugoniot pressures $P_H^{(i)}$ for those energies are calculated in PH. The corresponding volume changes are calculated using

$$I - I_0 = \frac{(P + P_0)(V_0 - V)}{2} \quad , \tag{4}$$

and the function g is given by

$$g(U) = P_H^{(1)} - P_H^{(2)} \quad . \tag{5}$$

```
      FUNCTION PH(XIH,I,J)                                                  PH          2
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,             PARAM       2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                      PARAM       3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                        PARAM       4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                            PARAM       5
      COMMON/CELL/R(MCL),U(MCL),V(MCL),XI(MCL),                             MCELL       2
     +P(MCL),SX(MCL),SZ(MCL),EE(MCL),T(MCL),Q(MCL),XM(MCL),IFLAG(MCL)       MCELL       3
     +,W(MCL)                                                               MCELL       4
      LEVEL 2,R                                                             MCELL       5
      COMMON/OVL/NDF,NI,NP,NG,TEND,TP(ML),TG(ML),UI,UF,UII,UFI,NADD,NM,     MCELL       6
     +IALPH,NDELT,LABEL(8),NDUMP,IDMP,NM1,TD(ML),IJK                        MCELL       7
      COMMON/MISC/TIME,ICYCL,DT,NCL,IA,BU,BUI,F2,F3,JS                      MCELL       8
      LEVEL 2,TIME                                                          MCELL       9
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO     INIT        2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML),    INIT        3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)                INIT        4
      COMMON/RLC/RC(ML),RP(ML),RLV(ML),PH1,DV1,DV2                          RLC         2
      COMMON/VOID/INTX(ML2),JV(ML2),IV(ML2),NNV                             VD          2
      COMMON/USUPC/C1(ML),S1(ML),C2(ML),S2(ML),SWV(ML),VMN(ML),             US          2
     +GAMMA(ML),ALP(ML)                                                     US          3
      COMMON/EOSN/IEOS(ML),ME(ML)                                           EN          2
      COMMON/ES/IE(ML2),NME                                                 ESM         2
      II=IE(I)                                                              PH         11
      JM=JV(I)-1                                                            PH         12
      IS=IEOS(I)                                                            PH         13
      GO TO (1,2,2,2),IS                                                    PH         14
    1 CONTINUE   USUP EOS                                                   PH         15
      C=C1(II)                                                              PH         16
      S=S1(II)                                                              PH         17
      UP=SQRT(2*(XIH-XI(J)))                                                PH         18
      VP=VO(II)*(1.-UP/(C+S*UP))  Volume on Hugoniot for Up                 PH         19
      IF(VP.LT.VMN(II).OR.VP.LT.SWV(II))GO TO 2                             PH         20
      PH=UP*(C+S*UP)/VO(II)  Hugoniot pressure                              PH         21
      GO TO 10                                                              PH         22
    2 CONTINUE                                                              PH         23
C     GENERAL EOS   ITERATE TO FIND HUGONIOT                                PH         24
      DVB=.01*V(J)                                                          PH         25
      DVC=2*DVB                                                             PH         26
      VI=V(J)-DVB                    Initialize                             PH         27
      CALL PTEOS(I,PH,TI,VI,XIH)                                            PH         28
      GB=PH-2*XIH/DVB                                                       PH         29
      IC=0                                                                  PH         30
   20 CONTINUE                                                              PH         31
      IC=IC+1                                                               PH         32
      IF(IC.GT.100)GO TO 99                                                 PH         33
      DVA=DVB                                                               PH         34
      GA=GB                                                                 PH         35
      DVB=DVC                                                               PH         36
      VI=V(J)-DVC                    Secant method iteration                PH         37
      CALL PTEOS(I,PH,TI,VI,XIH)                                            PH         38
      GB=PH-2*XIH/DVB                                                       PH         39
      DVC=(GB*DVA-GA*DVB)/(GB-GA)                                           PH         40
      IF(ABS((DVC-DVB)/DVC).GT.0.001)GO TO 20                               PH         41
   10 CONTINUE                                                              PH         42
      RETURN                                                                PH         43
   99 CONTINUE                                                              PH         44
      PRINT 990                                                             PH         45
  990 FORMAT(35H WARNING: FAILURE TO CONVERGE IN PH )                       PH         46
      RETURN                                                                PH         47
      END                                                                   PH         48
```

For a given specific internal energy, the volume on the Hugoniot and the Hugoniot pressure are determined.

Local Variables

II = IE(I) = original region #.

IS = IEOS(I) = EOS type.

C,S = in USUP fit $U_S = C + SU_P$.

UP = U_P = particle velocity relative to unshocked material.

VP = V_H from USUP EOS.

PH = P_H = calculated pressure in the iteration to find the Hugoniot pressure.

DVA,DVB,DVC = ΔV_{i-1}, ΔV_i, ΔV_{i+1}.

VI = V_i.

GA,GB = g_{i-1}, g_i ; $g = P_H - \frac{2\Delta I}{\Delta V}$, g is 0 for the Hugoniot.

IC = iteration count.

Notes

The USUP fit is treated as a special case because the Hugoniot pressure can be calculated directly as a function of the particle velocity , UP. The material is assumed to be in the initial state in order to allow this simplification. The error involved in this assumption should be small. The particle velocity is calculated using

$$\Delta I = \frac{U_P^2}{2} \quad . \tag{1}$$

From the jump condition for conservation of mass,

$$\rho_0 U_S = \rho(U_S - U_P) \quad , \tag{2}$$

we have, with a little algebra,

$$V = \left(1 - \frac{U_P}{U_S}\right) V_0 \quad . \tag{3}$$

The jump condition for conservation of momentum,

$$P_H = P_0 + \rho_0 U_S U_P \quad , \tag{4}$$

directly gives the Hugoniot pressure in terms of U_P provided a USUP fit is used, i.e.,

$$P_H = P_0 + \rho_0 U_P (C + S U_P) \quad . \tag{5}$$

However, if the final volume in Eq. (3) is small enough that the initial USUP fit is not used in the USUP EOS, then the general Hugoniot iteration scheme described below is used.

For a general EOS, we define a function, g(I,V) such that it is zero everywhere along the Hugoniot, i.e.,

$$g = P(I,V) - 2 \frac{I - I_0}{V_0 - V} + P_0 \quad , \tag{6}$$

which, as can be seen from the jump condition,

$$I - I_0 = \frac{(P + P_0)(V_0 - V)}{2} \quad , \tag{7}$$

satisfies the condition that g(I,V) is zero on the Hugoniot. In this subroutine, the specific internal energy I is given. So we are looking for the zero of g as a function of V only. The secant method,

$$\Delta V_{i+1} = \frac{\Delta V_{i-1} g_i - \Delta V_i g_{i-1}}{g_i - g_{i-1}} \quad , \tag{8}$$

is used with the initial values

$$\Delta V_0 = 0.01 \, V_0 \tag{9}$$

and

$$\Delta V_1 = 0.02 \, V_0 \quad , \tag{10}$$

where

$$\Delta V = V_0 - V \quad . \tag{11}$$

Iteration is allowed for a maximum of 100 cycles with a relative convergence criteria of 10^{-3} in ΔV.

E. SESAME Tabular Equation-of-State Subroutines

The following set of subroutines are used for reading and interpolating the SESAME equation-of-state tables. Further information may be found in Sec. VI.B.

```
      SUBROUTINE MATCHK(MID,NRS,LOC,TBLS,IFLG)                          SESAME      2
C-----------------------------------------------------------------------  SESAME      3
C                                                                         SESAME      4
C  SUBROUTINE  MATCHK(MID,NRS,LOC,TBLS,IFLG)                              SESAME      5
C                                                                         SESAME      6
C  PURPOSE     TO CHECK IF A MATERIAL HAS BEEN                            SESAME      7
C              PREVIOUSLY LOADED                                          SESAME      8
C                                                                         SESAME      9
C  ARGUMENTS   MID        (INPUT)   SESAME MATERIAL ID                   SESAME     10
C              NRS        (INPUT)   NUMBER OF REGIONS                    SESAME     11
C              LOC        (INPUT)   ARRAY OF FIRST WORD LOCATIONS        SESAME     12
C                                   IN TABLE STORAGE ARRAY FOR            SESAME     13
C                                   FOR EACH REGION                       SESAME     14
C              TBLS       (INPUT)   TABLE STORAGE ARRAY                  SESAME     15
C              IFLG       (OUTPUT)  =0 MATERIAL NOT PREVIOUSLY LOADED    SESAME     16
C                                   GT.0 LOCATION OF TABLE IF LOADED      SESAME     17
C                                   ALREADY                               SESAME     18
C                                                                         SESAME     19
C  REMARKS     NONE                                                       SESAME     20
C                                                                         SESAME     21
C  EXTERNALS   NONE                                                       SESAME     22
C                                                                         SESAME     23
C  PROGRAMMER  J.ABDALLAH,JR.                                             SESAME     24
C                                                                         SESAME     25
C  DATE        26 APRIL 1979                                              SESAME     26
C                                                                         SESAME     27
C-----------------------------------------------------------------------  SESAME     28
      LEVEL 2,TBLS                                                        SESAME     29
      DIMENSION LOC(1),TBLS(1)                                            SESAME     30
      IFLG=0                                                              SESAME     31
      DO 100 J=1,NRS                                                      SESAME     32
      LC=LOC(J)                                                           SESAME     33
      IF(LC.LE.0) GO TO 100                                               SESAME     34
      ITEST=TBLS(LC)                                                      SESAME     35
      IF(MID.EQ.ITEST) GO TO 200                                          SESAME     36
  100 CONTINUE                                                            SESAME     37
      RETURN                                                              SESAME     38
  200 IFLG=LC                                                             SESAME     39
      RETURN                                                              SESAME     40
      END                                                                 SESAME     41
```

```
      SUBROUTINE TABFCH(MID,TID,LIB,A,LEN,IFLAG)                        SESAME     42
C-----------------------------------------------------------------------SESAME     43
C                                                                       SESAME     44
C  SUBROUTINE  TABFCH(MID,TID,LIB,A,LEN,IFLAG)                          SESAME     45
C                                                                       SESAME     46
C  PURPOSE     TO FETCH A GIVEN TABLE FOR A GIVEN MATERIAL              SESAME     47
C              FROM A SESAME II LIBRARY                                 SESAME     48
C                                                                       SESAME     49
C  ARGUMENTS   MID        (INPUT)   MATERIAL ID                        SESAME     50
C              TID        (INPUT)   TABLE NO.- IF 0.0 MATERIAL INDEX   SESAME     51
C                                   IS RETURNED                         SESAME     52
C              LIB        (INPUT)   LIBRARY FILE UNIT NO.              SESAME     53
C              A          (OUTPUT)  ARRAY FOR TABLE STORAGE            SESAME     54
C              LEN        (INPUT)   NO. OF WORDS IN A AVAILABLE        SESAME     55
C              IFLAG      (OUTPUT)  =0 IF TABLE COULD NOT BE LOCATED   SESAME     56
C                                   GT. 0=NO. OF WORDS IN TABLE RETURNED SESAME   57
C                                   LT. 0 - NO. OF ADDITIONAL           SESAME     58
C                                   WORDS NEEDED                        SESAME     59
C                                                                       SESAME     60
C  REMARKS     A RANDOM I/O TECHNIQUE IS USED TO LOCATE AND LOAD        SESAME     61
C              THE SPECIFIED TABLE FROM THE SESAME II LIBRARY.          SESAME     62
C              THE MATERIAL INDEX AND ITS ADDRESS ARE TO SAVED          SESAME     63
C              TO HASTEN THE FETCHING OF ANOTHER TABLE FOR THE SAME     SESAME     64
C              MATERIAL AND LIBRARY FILE IN SUBSEQUENT CALLS TO         SESAME     65
C              TABFCH.                                                  SESAME     66
C                                                                       SESAME     67
C  EXTERNALS   INBUFR                                                   SESAME     68
C                                                                       SESAME     69
C  PROGRAMMER  J.ABDALLAH.,JR.                                          SESAME     70
C                                                                       SESAME     71
C  DATE        24 APRIL 1979                                            SESAME     72
C                                                                       SESAME     73
C-----------------------------------------------------------------------SESAME     74
      LEVEL 2,A                                                         SESAME     75
      DIMENSION A(1),HINDEX(35)                                         SESAME     76
      DATA HINDEX(1)/0.0/                                               SESAME     77
      DATA LIBLST/0/                                                    SESAME     78
      IFLAG=0                                                           SESAME     79
C . . FIND NO. MATERIALS ON LIBRARY                                     SESAME     80
      IF(LIB.NE.LIBLST) GO TO 50                                        SESAME     81
      IDLAST=HINDEX(1)                                                  SESAME     82
      IF(IDLAST.EQ.MID) GO TO 230                                       SESAME     83
 50   LIBLST=LIB                                                        SESAME     84
      NW=1                                                              SESAME     85
      IF(LEN.LT.NW) GO TO 999                                           SESAME     86
      CALL INBUFR(LIB,A,1,1,IER)                                        SESAME     87
      N=A(1)                                                            SESAME     88
      NW=N+N+N                                                          SESAME     89
      IF(LEN.LT.NW) GO TO 999                                           SESAME     90
      CALL INBUFR(LIB,A,NW,5,IER)                                       SESAME     91
C . . FIND ADDRESS OF MATERIAL FILE                                     SESAME     92
      DO 100 J=1,N                                                      SESAME     93
      ITEST=A(J)                                                        SESAME     94
      IF(ITEST.NE.MID) GO TO 100                                        SESAME     95
      NW=A(J+N)                                                         SESAME     96
      IAD=A(J+N+N)                                                      SESAME     97
      GO TO 200                                                         SESAME     98
 100  CONTINUE                                                          SESAME     99
      RETURN                                                            SESAME    100
C . . GET MATERIAL INDEX                                                SESAME    101
```

```
 200  IF(LEN.LT.NW) GO TO 999                                  SESAME    102
      IADX=IAD                                                 SESAME    103
      CALL INBUFR(LIB,A,NW,IADX,IER)                           SESAME    104
      DO 210 J=1,NW                                            SESAME    105
      HINDEX(J)=A(J)                                           SESAME    106
 210  CONTINUE                                                 SESAME    107
      IF(TID.EQ.0.0) GO TO 500                                 SESAME    108
 230  N=HINDEX(5)                                              SESAME    109
      IAD=IADX+6+N+N                                           SESAME    110
      DO 300 J=1,N                                             SESAME    111
      NW=HINDEX(5+J+N)                                         SESAME    112
      IF(TID.NE.HINDEX(5+J)) GO TO 250                         SESAME    113
      GO TO 400                                                SESAME    114
 250  IAD=IAD+NW+1                                             SESAME    115
 300  CONTINUE                                                 SESAME    116
      RETURN                                                   SESAME    117
 400  IF(LEN.LT.NW) GO TO 999                                  SESAME    118
C . . READ REQUESTED TABLE                                     SESAME    119
      CALL INBUFR(LIB,A,NW,IAD,IER)                            SESAME    120
 500  IFLAG=NW                                                 SESAME    121
      RETURN                                                   SESAME    122
 999  IFLAG=LEN-NW                                             SESAME    123
      RETURN                                                   SESAME    124
      END                                                      SESAME    125
```

```
      SUBROUTINE INBUFR(LU,Z,NW,IAD,IFLG)                                SESAME    126
C-----------------------------------------------------------------------  SESAME    127
C                                                                          SESAME    128
C  SUBROUTINE  INBUFR(LU,Z,NW,IAD,IFLG)                                    SESAME    129
C                                                                          SESAME    130
C  PURPOSE     RANDOM I/O READ                                             SESAME    131
C                                                                          SESAME    132
C  ARGUMENTS   LU    (INPUT)  UNIT NO.                                     SESAME    133
C              Z     (OUTPUT)  STORAGE AREA WHERE DAT IS RETURNED          SESAME    134
C              NW    (INPUT)  NO. OF WORDS TO BE READ                      SESAME    135
C              IAD   (INPUT)  STARTING DISK ADDRESS OF DATA                SESAME    136
C              IFLG  (OUTPUT) 0=NORMAL                                     SESAME    137
C                              1=EOF ENCOUNTERED                           SESAME    138
C                             -1=ERROR                                     SESAME    139
C                                                                          SESAME    140
C  REMARKS     NONE                                                        SESAME    141
C                                                                          SESAME    142
C  EXTERNALS   RDISK                                                       SESAME    143
C                                                                          SESAME    144
C  PROGRAMMER  J.ABDALLAH,JR.                                              SESAME    145
C                                                                          SESAME    146
C  DATE        1 MAY 1979                                                  SESAME    147
C                                                                          SESAME    148
C-----------------------------------------------------------------------  SESAME    149
      LEVEL 2,Z                                                            SESAME    150
      CALL RDISK(LU,Z,NW,IAD)                                              SESAME    151
      IF(UNIT(LU)) 10,20,30                                                SESAME    152
 10   IFLG=1                                                               SESAME    153
      RETURN                                                               SESAME    154
 20   IFLG=0                                                               SESAME    155
      RETURN                                                               SESAME    156
 30   IFLG=-1                                                              SESAME    157
      RETURN                                                               SESAME    158
      END                                                                  SESAME    159
```

```
      FUNCTION DPACK(A,B)                                                SESAME    160
C-----------------------------------------------------------------------SESAME    161
C                                                                       SESAME    162
C  FUNCTION   DPACK                                                    SESAME    163
C                                                                       SESAME    164
C  PURPOSE    TO DOUBLE PACK ARGUMENTS A AND B INTO A SINGLE WORD      SESAME    165
C                                                                       SESAME    166
C  REMARKS    SYSTEM DEPENDENT SHIFT FUNCTION                          SESAME    167
C                                                                       SESAME    168
C  PROGRAMMER  J.ABDALLAH,JR.                                          SESAME    169
C                                                                       SESAME    170
C  DATE        1 MAY 1979                                               SESAME    171
C                                                                       SESAME    172
C-----------------------------------------------------------------------SESAME    173
      EQUIVALENCE (I1,X1),(I2,X2)                                       SESAME    174
      DATA MASK/777777777700000000008/                                  SESAME    175
      X1=A                                                              SESAME    176
      X2=B                                                              SESAME    177
      I1=I1.AND.MASK                                                    SESAME    178
      I2=I2.AND.MASK                                                    SESAME    179
      I2=SHIFT(I2,30)                                                   SESAME    180
      I1=I1.OR.I2                                                       SESAME    181
      DPACK=X1                                                          SESAME    182
      RETURN                                                            SESAME    183
      END                                                               SESAME    184
```

```
      FUNCTION ISRCHK(X,TBLS,N,K,NSFT)                                  SESAME    185
C-----------------------------------------------------------------------SESAME    186
C                                                                       SESAME    187
C  FUNCTION:    ISRCHK(X,TBLS,N,K,NSFT)                                 SESAME    188
C                                                                       SESAME    189
C  PURPOSE:     FIND INDEX OF X IN AN ARRAY TBLS.  TABLE VALUES         SESAME    190
C               NEED NOT BE CONTIGUOUS AND CAN BE IN EITHER             SESAME    191
C               ASCENDING OR DESCENDING ORDER.                          SESAME    192
C                                                                       SESAME    193
C  ARGUMENTS:   X     (INPUT) - VALUE TO BE LOCATED                     SESAME    194
C               TBLS  (INPUT) - TABLE TO BE SEARCHED                    SESAME    195
C               N     (INPUT) - NUMBER OF VALUES TO BE SEARCHED         SESAME    196
C               K     (INPUT) - SPACING BETWEEN VALUES IN TABLE         SESAME    197
C               THE VALUE OF THE FUNCTION = INDEX I, WHERE              SESAME    198
C                 TBLS(1+K*(I-1)).LE.X.LT.TBLS(1+K*I), OR               SESAME    199
C                 TBLS(1+K*(I-1)).GE.X.GT.TBLS(1+K*I), OR               SESAME    200
C                 I=0 OR I=N IF X IS OUTSIDE RANGE OF TABLE.            SESAME    201
C               NSFT  (INPUT) - NO. OF BITS THE TABLE VALUES ARE        SESAME    202
C                               TO BE SHIFTED                           SESAME    203
C                                                                       SESAME    204
C  REMARKS:     TBLS CAN BE DECLARED LCM ON THE CDC 7600.               SESAME    205
C                                                                       SESAME    206
C  EXTERNALS:   SHIFT.                                                  SESAME    207
C                                                                       SESAME    208
C  PROGRAMMER:  G. I. KERLEY, T-4., J.ABDALLAH,JR.                      SESAME    209
C                                                                       SESAME    210
C  DATE:        19 NOVEMBER 1976,REVISED 6 JULY 1979                    SESAME    211
C                                                                       SESAME    212
C-----------------------------------------------------------------------SESAME    213
      LEVEL 2,TBLS                                                      SESAME    214
      DIMENSION TBLS(1)                                                 SESAME    215
      ISRCHK = 0                                                        SESAME    216
      J = N+1                                                           SESAME    217
      KI = 1-K                                                          SESAME    218
      S1=TBLS(1)                                                        SESAME    219
      S1=SHIFT(S1,NSFT)                                                 SESAME    220
      S=TBLS(KI+K*N)                                                    SESAME    221
      S=SHIFT(S,NSFT)                                                   SESAME    222
      S=S-S1                                                            SESAME    223
 1    IF(J-ISRCHK.EQ.1) RETURN                                          SESAME    224
      JP = .5*(J+ISRCHK)                                                SESAME    225
      S1=TBLS(KI+K*JP)                                                  SESAME    226
      S1=SHIFT(S1,NSFT)                                                 SESAME    227
      IF(S*(X-S1).LT.0.0) GO TO 2                                       SESAME    228
      ISRCHK = JP                                                       SESAME    229
      GO TO 1                                                           SESAME    230
 2    J = JP                                                            SESAME    231
      GO TO 1                                                           SESAME    232
      END                                                               SESAME    233
```

```
      SUBROUTINE T4INTP                                                 SESAME    234
C-----------------------------------------------------------------------SESAME    235
C                                                                       SESAME    236
C  SUBROUTINE:  T4INTP                                                  SESAME    237
C                                                                       SESAME    238
C  PURPOSE:     INTERPOLATE FOR A FUNCTION Z(X,Y) AND ITS               SESAME    239
C               DERIVATIVES FROM TABLES LOCATED IN ARRAY TBLS.          SESAME    240
C                                                                       SESAME    241
C               THE ROUTINE REQUIRES COMMON BLOCKS,                     SESAME    242
C               COMMON/RTBLK2/LOCX,IX,NX,LOCY,IY,NY,LOCZ,NZ,NSFT,       SESAME    243
C                            X,Y,Z(3),IP,IDS,ZZ                         SESAME    244
C                 LOCX = LOCATION OF X VECTOR                           SESAME    245
C                 IX   = INDEX OF X VECTOR                              SESAME    246
C                 NX   = LENGTH OF X VECTOR                             SESAME    247
C                 LOCY = LOCATION OF Y VECTOR                           SESAME    248
C                 IY   = INDEX OF Y VECTOR                              SESAME    249
C                 NY   = LENGTH OF Y VECTOR                             SESAME    250
C                 LOCZ = LOCATION OF Z(X,Y) ARRAY                       SESAME    251
C                 NZ   = SPACING OF Z ARRAY                             SESAME    252
C                 NSFT = BIT SHIFT PARAMETER                            SESAME    253
C               X,Y  (INPUT) - INDEPENDENT VARIABLES                    SESAME    254
C               Z    (OUTPUT) - VECTOR OF LENGTH 3, WHERE               SESAME    255
C                 Z(1) = VALUE OF FUNCTION                              SESAME    256
C                 Z(2) = X DERIVATIVE OF FUNCTION                       SESAME    257
C                 Z(3) = Y DERIVATIVE OF FUNCTION                       SESAME    258
C               ZZ   (IN/OUT) - COEFFICIENT VECTOR OF LENGTH 16         SESAME    259
C               IP    (INPUT) - BRANCH PARAMETER                        SESAME    260
C                 IP.EQ.0, USE INPUT COEFFICIENTS IN ZZ                 SESAME    261
C                 IP.NE.0, CALCULATE ZZ VECTOR FIRST                    SESAME    262
C               IDS  (INPUT) - DISPLACEMENT INTO ZZ FOR COEFFS.         SESAME    263
C                              TO BE USED                               SESAME    264
C               COMMON/INTORD/IFN.                                      SESAME    265
C               IFN  (INPUT) - INTERPOLATION TYPE                       SESAME    266
C                 IFN.NE.1, RATIONAL FUNCTION                           SESAME    267
C                 IFN.EQ.1, BILINEAR                                    SESAME    268
C               COMMON/SESDAT/TBLS                                      SESAME    269
C                 TBLS IS THE TABLE STORAGE ARRAY                       SESAME    270
C                                                                       SESAME    271
C                                                                       SESAME    272
C  REMARKS:     UNLESS BILINEAR FORM IS SPECIFIED, ROUTINE              SESAME    273
C               USES RATIONAL FUNCTION METHOD WITH QUADRATIC            SESAME    274
C               ESTIMATE OF DERIVATIVES AT THE MESH POINTS.             SESAME    275
C               TBLS CAN BE DECLARED LCM ON THE CDC 7600.               SESAME    276
C                                                                       SESAME    277
C        *****  SYSTEM DEPENDENT FEATURE.  THE Z-ARRAY CAN BE           SESAME    278
C        *****  DOUBLE PACKED.  PARAMETER NSFT SPECIFIES THE            SESAME    279
C        *****  NUMBER OF BITS TO BE SHIFTED WHEN UNPACKING THE         SESAME    280
C        *****  RIGHT HALF OF THE WORD.  THIS ROUTINE USES              SESAME    281
C        *****  THE LASL SHIFT FUNCTION                                 SESAME    282
C                                                                       SESAME    283
C  EXTERNALS:   NONE, BUT A SEARCH ROUTINE MUST BE CALLED               SESAME    284
C               FIRST, TO COMPUTE INDICES IX AND IY.                    SESAME    285
C                                                                       SESAME    286
C  PROGRAMMER:  G. I. KERLEY, T-4., J. ABDALLAH,T-4.                    SESAME    287
C                                                                       SESAME    288
C  DATE:        01 AUG 1979                                             SESAME    289
C                                                                       SESAME    290
C-----------------------------------------------------------------------SESAME    291
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM       2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM       3
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     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM      4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                        PARAM      5
      LEVEL 2,TBLS                                                      SESAME   293
      COMMON/RTBLK2/LOCX,IX,NX,LOCY,IY,NY,LOCZ,NZ,NSFT,X,Y,Z(3),        SESAME   294
     $ IP,IDS,ZZ(32)                                                    SESAME   295
      COMMON/INTORD/IFN                                                 SESAME   296
      COMMON/SESDAT/TBLS(NSD)                                           SESAME   297
C  CALCULATE COEFFICIENTS FOR RATIONAL FUNCTION INTERPOLATION           SESAME   298
      IF(IFN.EQ.1) GO TO 13                                             SESAME   299
      IF(IP.EQ.0) GO TO 8                                               SESAME   300
      I = LOCX+IX-1                                                     SESAME   301
      IZ = LOCZ+NZ*(IX-1+NX*(IY-1))                                     SESAME   302
      KZ = NZ                                                           SESAME   303
      IBR = IX                                                          SESAME   304
      NBR = NX-IX                                                       SESAME   305
      ZZ(IDS+4) = TBLS(I)                                               SESAME   306
      DO 7 K=1,4                                                        SESAME   307
      KI=IDS+K-1                                                        SESAME   308
      IF(K.LT.4) GO TO 1                                                SESAME   309
      IZ = IZ+NZ                                                        SESAME   310
      GO TO 4                                                           SESAME   311
1     IF(K.LT.3) GO TO 2                                                SESAME   312
      ZZ(IDS+6) = D                                                     SESAME   313
      I = LOCY+IY-1                                                     SESAME   314
      KZ = KZ*NX                                                        SESAME   315
      IZ = IZ-KZ                                                        SESAME   316
      IBR = IY                                                          SESAME   317
      NBR = NY-IY                                                       SESAME   318
      ZZ(IDS+5) = TBLS(I)                                               SESAME   319
      GO TO 3                                                           SESAME   320
2     IF(K.LT.2) GO TO 3                                                SESAME   321
      IZ = IZ+NX*NZ                                                     SESAME   322
      GO TO 4                                                           SESAME   323
3     D = TBLS(I+1)-TBLS(I)                                             SESAME   324
4     ZZ(KI)=SHIFT(TBLS(IZ),NSFT)                                       SESAME   325
      S=SHIFT(TBLS(IZ+KZ),NSFT)                                         SESAME   326
      S = (S-ZZ(KI))/D                                                  SESAME   327
      IF(NBR.EQ.1) GO TO 5                                              SESAME   328
      SP=SHIFT(TBLS(IZ+KZ+KZ),NSFT)                                     SESAME   329
      SP = (SP-D*S-ZZ(KI))/(TBLS(I+2)-TBLS(I+1))                        SESAME   330
      G2 = (SP-S)/(TBLS(I+2)-TBLS(I))                                   SESAME   331
      IF(IBR.GT.1) GO TO 5                                              SESAME   332
      IF(S*(S-D*G2).LE.0.) G2=S/D                                       SESAME   333
      G1 = G2                                                           SESAME   334
      GO TO 6                                                           SESAME   335
5     DM = TBLS(I)-TBLS(I-1)                                            SESAME   336
      SM=SHIFT(TBLS(IZ-KZ),NSFT)                                        SESAME   337
      SM = (ZZ(KI)-SM)/DM                                               SESAME   338
      G1 = (S-SM)/(D+DM)                                                SESAME   339
      IF(NBR.EQ.1) G2=G1                                                SESAME   340
      IF(IBR.GT.2) GO TO 6                                              SESAME   341
      IF(SM*(SM-DM*G1).LE.0.) G1=(S-SM-SM)/D                            SESAME   342
6     IF(G2.NE.0.) G1=G1/G2                                             SESAME   343
      ZZ(KI+8) = G1                                                     SESAME   344
7     ZZ(KI+12) = G2                                                    SESAME   345
      ZZ(IDS+7)=D                                                       SESAME   346
      ZZ8=ZZ(IDS+7)                                                     SESAME   347
      ZZ7=ZZ(IDS+6)                                                     SESAME   348
      ZZ(IDS+2)=(ZZ(IDS+1)-ZZ(IDS))/ZZ8                                 SESAME   349
      ZZ(IDS+1)=(ZZ(IDS+3)-ZZ(IDS))/ZZ7                                 SESAME   350
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      ZZ(IDS+3)=(S-ZZ(IDS+2))/ZZ7                                        SESAME    351
      ZZ(IDS+12)=ZZ(IDS+12)/ZZ8                                          SESAME    352
      ZZ(IDS+13)=ZZ(IDS+13)/ZZ8                                          SESAME    353
      ZZ(IDS+14)=ZZ(IDS+14)/ZZ7                                          SESAME    354
      ZZ(IDS+15)=ZZ(IDS+15)/ZZ7                                          SESAME    355
C  EVALUATE RATIONAL FUNCTION FROM PRECALCULATED COEFFICIENTS            SESAME    356
 8    QX = X-ZZ(IDS+4)                                                   SESAME    357
      RX = ZZ(IDS+6)-QX                                                  SESAME    358
      QY = Y-ZZ(IDS+5)                                                   SESAME    359
      RY = ZZ(IDS+7)-QY                                                  SESAME    360
      IF(RX.NE.0.) GO TO 9                                               SESAME    361
      W1 = 1.                                                            SESAME    362
      W2 = 1.                                                            SESAME    363
      GO TO 10                                                           SESAME    364
 9    W1 = 1.-1./(1.+ABS(ZZ(IDS+8)*QX/RX))                               SESAME    365
      W2 = 1.-1./(1.+ABS(ZZ(IDS+9)*QX/RX))                               SESAME    366
 10   F1 = ZZ(IDS+12)*(W1+ZZ(IDS+8)*(1.-W1))                             SESAME    367
      F2 = ZZ(IDS+13)*(W2+ZZ(IDS+9)*(1.-W2))                             SESAME    368
      Z(2) = ZZ(IDS+6)*(RY*(F1-ZZ(IDS+12))*W1+QY*(F2-ZZ(IDS+13))*W2)     SESAME    369
      G1 = RY*F1+QY*F2                                                   SESAME    370
      IF(RY.NE.0) GO TO 11                                               SESAME    371
      W1 = 1.                                                            SESAME    372
      W2 = 1.                                                            SESAME    373
      GO TO 12                                                           SESAME    374
11    W1 = 1.-1./(1.+ABS(ZZ(IDS+10)*QY/RY))                              SESAME    375
      W2 = 1.-1./(1.+ABS(ZZ(IDS+11)*QY/RY))                              SESAME    376
 12   F3 = ZZ(IDS+14)*(W1+ZZ(IDS+10)*(1.-W1))                            SESAME    377
      F4 = ZZ(IDS+15)*(W2+ZZ(IDS+11)*(1.-W2))                            SESAME    378
      Z(3) = ZZ(IDS+7)*(RX*(F3-ZZ(IDS+14))*W1+QX*(F4-ZZ(IDS+15))*W2)     SESAME    379
      G2 = RX*F3+QX*F4                                                   SESAME    380
      ZZ2=ZZ(IDS+1)                                                      SESAME    381
      ZZ3=ZZ(IDS+2)                                                      SESAME    382
      ZZ4=ZZ(IDS+3)                                                      SESAME    383
      Z(1) = ZZ(IDS)+(ZZ2+ZZ4*QY-RX*G1)*QX+(ZZ3-RY*G2)*QY                SESAME    384
      Z(2) = Z(2)+ZZ2+QY*(ZZ4+RY*(F3-F4))+(QX-RX)*G1                     SESAME    385
      Z(3) = Z(3)+ZZ3+QX*(ZZ4+RX*(F1-F2))+(QY-RY)*G2                     SESAME    386
      RETURN                                                             SESAME    387
C  CALCULATE COEFFICIENTS FOR BILINEAR INTERPOLATION                     SESAME    388
 13   IF(IP.EQ.0) GO TO 14                                               SESAME    389
      I=LOCX+IX                                                          SESAME    390
      IND=IDS+4                                                          SESAME    391
      ZZ(IND)=TBLS(I-1)                                                  SESAME    392
      DX=TBLS(I)-ZZ(IND)                                                 SESAME    393
      J=LOCY+IY                                                          SESAME    394
      IND=IDS+5                                                          SESAME    395
      ZZ(IND)=TBLS(J-1)                                                  SESAME    396
      DY=TBLS(J)-ZZ(IND)                                                 SESAME    397
      IZ=LOCZ+NZ*(IX-1+NX*(IY-1))                                        SESAME    398
      ZZ(IDS)=SHIFT(TBLS(IZ),NSFT)                                       SESAME    399
      IND=IDS+1                                                          SESAME    400
      ZZ(IND)=SHIFT(TBLS(IZ+NZ),NSFT)                                    SESAME    401
      ZZ(IND)=(ZZ(IND)-ZZ(IDS))/DX                                       SESAME    402
      IZ=IZ+NZ*NX                                                        SESAME    403
      IND=IDS+2                                                          SESAME    404
      ZZ(IND)=SHIFT(TBLS(IZ),NSFT)                                       SESAME    405
      ZZ(IND)=(ZZ(IND)-ZZ(IDS))/DY                                       SESAME    406
      IND=IDS+3                                                          SESAME    407
      ZZ(IND)=SHIFT(TBLS(IZ+NZ),NSFT)                                    SESAME    408
      ZZ(IND)=(ZZ(IND)-ZZ(IDS)-ZZ(IDS+1)*DX-ZZ(IDS+2)*DY)/(DX*DY)       SESAME    409
C  EVALUATE BILINEAR FUNCTION FROM PRECALCULATED COEFFICIENTS             SESAME    410
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14    QX = X-ZZ(IDS+4)                                          SESAME    411
      QY = Y-ZZ(IDS+5)                                          SESAME    412
      Z(2) = ZZ(IDS+1)+ZZ(IDS+3)*QY                             SESAME    413
      Z(3) = ZZ(IDS+2)+ZZ(IDS+3)*QX                             SESAME    414
      Z(1) = ZZ(IDS)+Z(2)*QX+ZZ(IDS+2)*QY                       SESAME    415
      RETURN                                                    SESAME    416
      END                                                       SESAME    417
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      SUBROUTINE GETINV(IR,MID,IDT,TBLS,LCNT,LU,IFL,ZB)                  SESAME    418
C-----------------------------------------------------------------------  SESAME    419
C                                                                         SESAME    420
C  SUBROUTINE  GETINV(IR,MID,IDT,TBLS,LCNT,LU,IFL,ZB)                     SESAME    421
C                                                                         SESAME    422
C  PURPOSE     TO LOAD INVERTED (ENERGY BASED) SESAME II                  SESAME    423
C              ECS TABLES                                                 SESAME    424
C                                                                         SESAME    425
C  ARGUMENTS   IR         (INPUT)   REGION NO.                            SESAME    426
C              MID        (INPUT)   SESAME MATERIAL ID                    SESAME    427
C              IDT        (INPUT)   DATA TYPE INDICATOR                   SESAME    428
C              TBLS       (INPUT)   TABLE STORAGE ARRAY                   SESAME    429
C              LCNT       (IN/OUT)  POSITION IN ARRAY FOR STORING TABLES  SESAME    430
C              LU         (INPUT)   SESAME LIBRARY UNIT NO.               SESAME    431
C              IFL        (OUTPUT)  ERROR FLAG                            SESAME    432
C                                   2=MATERIAL ALREADY LOADED             SESAME    433
C                                   1=SUCCESSFUL LOADING                  SESAME    434
C                                   0=DATA NOT FOUND                      SESAME    435
C                                   LT.0 FOR - THE NO. OF EXTRA WORDS     SESAME    436
C                                   NEEDED FOR LOADING                    SESAME    437
C              ZB         (OUTPUT)  ATOMIC CHARGE,CHARGE**2,AND MASS      SESAME    438
C                                   ZB(1)=Z                               SESAME    439
C                                   ZB(2)=Z**2                            SESAME    440
C                                   ZB(3)=A                               SESAME    441
C                                                                         SESAME    442
C  REMARKS     UNITS - ENERGY      MBAR*CC/GM                            SESAME    443
C                      TEMP        DEGREES KELVIN                        SESAME    444
C                      DENSITY     GRAMS/CC                              SESAME    445
C                      PRESSURE    MBAR                                  SESAME    446
C                                                                         SESAME    447
C  EXTERNALS   MATCHK,TABFCH,INV301                                       SESAME    448
C                                                                         SESAME    449
C  PROGRAMMER  J.ABDALLAH,JR.                                             SESAME    450
C                                                                         SESAME    451
C  DATE        13 JUNE 1979                                               SESAME    452
C                                                                         SESAME    453
C-----------------------------------------------------------------------  SESAME    454
C                                                                         SESAME    455
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,           PARAM       2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                    PARAM       3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                      PARAM       4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                          PARAM       5
      LEVEL 2,TBLS                                                       SESAME    457
      COMMON/S2DIR/LCMX,NRS,LCFW(ML,1)                                   SESAME    458
      DIMENSION ZB(3),TBLS(1)                                            SESAME    459
C . . UNIT CONVERSION FACTORS                                            SESAME    460
      DATA TFAC,RFAC,PEFAC/1.0,1.0,.01/                                  SESAME    461
      CALL MATCHK(MID,NRS,LCFW(1,IDT),TBLS(1),IFL)                       SESAME    462
      IF(IFL.EQ.0) GO TO 10                                              SESAME    463
      LCFW(IR,IDT)=IFL                                                   SESAME    464
      IFL=2                                                              SESAME    465
      RETURN                                                             SESAME    466
 10   NL=LCMX-LCNT-1                                                     SESAME    467
C . . FETCH EOS TABLES                                                   SESAME    468
      CALL TABFCH(MID,201.,LU,TBLS(LCNT+2),NL,IFL)                       SESAME    469
      IF(IFL.LE.0) RETURN                                                SESAME    470
      ZB(1)=TBLS(LCNT+2)                                                 SESAME    471
      ZB(2)=ZB(1)*ZB(1)                                                  SESAME    472
      ZB(3)=TBLS(LCNT+3)                                                 SESAME    473
      TBLS(LCNT+1)=TBLS(LCNT+4)                                          SESAME    474
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      CALL TABFCH(MID,301.,LU,TBLS(LCNT+2),NL,IFL)                    SESAME   475
      IF(IFL.LE.0) RETURN                                             SESAME   476
      TBLS(LCNT)=FLOAT(MID)                                           SESAME   477
      CALL PERTCB(IR,TBLS(LCNT),ZB(1),ZB(3))                          SESAME   478
      NR=TBLS(LCNT+2)                                                 SESAME   479
      NT=TBLS(LCNT+3)                                                 SESAME   480
      NRT=NR*NT                                                       SESAME   481
      LOCP=LCNT+3+NR+NT                                               SESAME   482
C . . CONVERT TO DESIRED UNITS                                        SESAME   483
      DO 30 I=1,NT                                                    SESAME   484
      TBLS(3+I+LCNT+NR)=TFAC*TBLS(3+I+LCNT+NR)                        SESAME   485
      DO 30 J=1,NR                                                    SESAME   486
      IF(I.GT.1) GO TO 20                                             SESAME   487
      TBLS(3+J+LCNT)=TBLS(3+J+LCNT)*RFAC                              SESAME   488
 20   LOCP=LOCP+1                                                     SESAME   489
      TBLS(LOCP)=PEFAC*TBLS(LOCP)                                     SESAME   490
      TBLS(LOCP+NRT)=PEFAC*TBLS(LOCP+NRT)                             SESAME   491
 30   CONTINUE                                                        SESAME   492
C . . WINDOW TABLES HERE AND RESET VALUES OF NR NT AND                SESAME   493
C     NRT IF WINDOWING IS NEEDED                                      SESAME   494
C . . INVERT TABLES                                                   SESAME   495
C . . CHECK TO SEE IF THERE IS ENOUGH ROOM TO INVERT THE TABLES       SESAME   496
C     NINV IS THE LAST LOCATION NEEDED FOR TABLE INVERSION            SESAME   497
      NINV=LCNT+3+2*NRT+2*NR+4*NT                                     SESAME   498
      IF(NINV.LE.LCMX) GO TO 40                                       SESAME   499
      IFL=LCMX-NINV                                                   SESAME   500
      RETURN                                                          SESAME   501
 40   RO=TBLS(LCNT+1)                                                 SESAME   502
      LOC=LCNT+2                                                      SESAME   503
      CALL INV301(TBLS,LOC,RO,LDS)                                    SESAME   504
C . . DOUBLE PACK DEPENDENT VARIABLES                                 SESAME   505
      LOCP=LCNT+3+NR+NT+NR                                            SESAME   506
      DO 50 I=1,NRT                                                   SESAME   507
      LOCP=LOCP+1                                                     SESAME   508
      PTEM=TBLS(LOCP)                                                 SESAME   509
      TTEM=TBLS(LOCP+NRT)                                             SESAME   510
      TBLS(LOCP)=DPACK(PTEM,TTEM)                                     SESAME   511
 50   CONTINUE                                                        SESAME   512
C . . WRAP UP                                                         SESAME   513
      LCFW(IR,IDT)=LCNT                                               SESAME   514
      LCNT=LCNT+2+LDS-NRT                                             SESAME   515
      IFL=1                                                           SESAME   516
      RETURN                                                          SESAME   517
      END                                                             SESAME   518
```

```
      SUBROUTINE RATFN1                                                 SESAME     519
C-----------------------------------------------------------------------SESAME     520
C                                                                       SESAME     521
C  SUBROUTINE:  RATFN1                                                  SESAME     522
C                                                                       SFSAME     523
C  PURPOSE:     INTERPOLATE FOR A FUNCTION Y(X) AND ITS                 SESAME     524
C               DERIVATIVE FROM TABLES LOCATED IN ARRAY TBLS.           SESAME     525
C                                                                       SESAME     526
C               THE ROUTINE ALSO REQUIRES COMMON BLOCKS,                SESAME     527
C               COMMON/RTBLK1/LOCX,KX,LOCY,KY,I,N,IP,X,Y(2)             SESAME     528
C                 LOCX = LOCATION OF X VECTOR                           SESAME     529
C                 KX   = SPACING OF X VECTOR                            SESAME     530
C                 LOCY = LOCATION OF Y VECTOR                           SESAME     531
C                 KY   = SPACING OF Y VECTOR                            SESAME     532
C                 I    = INDEX OF X AND Y VECTORS                       SESAME     533
C                 N    = LENGTH OF X AND Y VECTORS                      SESAME     534
C               X    (INPUT) - INDEPENDENT VARIABLE                     SESAME     535
C               Y   (OUTPUT) - VECTOR OF LENGTH 2, WHERE                SESAME     536
C                 Y(1) = VALUE OF FUNCTION                              SESAME     537
C                 Y(2) = DERIVATIVE OF FUNCTION                         SESAME     538
C               IP   (INPUT) - BRANCH PARAMETER                         SESAME     539
C                 IP.EQ.0, USE INPUT COEFFICIENTS IN YY                 SESAME     540
C                 IP.NE.0, CALCULATE YY VECTOR FIRST                    SESAME     541
C               COMMON/INTORD/IFN                                       SESAME     542
C               IFN  (INPUT) - INTERPOLATION TYPE                       SESAME     543
C                 IFN.NE.1, RATIONAL FUNCTION                           SESAME     544
C                 IFN.EQ.1, LINEAR                                      SESAME     545
C               COMMON/SESDAT/TBLS                                      SESAME     546
C                TBLS (INPUT) - TABLE STORAGE ARRAY                     SESAME     547
C                                                                       SESAME     548
C                                                                       SESAME     549
C  REMARKS:     UNLESS LINEAR FORM IS SPECIFIED, ROUTINE                SESAME     550
C               USES RATIONAL FUNCTION METHOD WITH QUADRATIC            SFSAME     551
C               ESTIMATE OF DERIVATIVES AT THE MESH POINTS.             SESAME     552
C               TBLS CAN BE DECLARED LCM ON THE CDC 7600.               SESAME     553
C                                                                       SESAME     554
C  EXTERNALS:   NONE, BUT A SEARCH ROUTINE MUST BE CALLED               SESAME     555
C               FIRST, TO COMPUTE INDEX I.                              SESAME     556
C                                                                       SESAME     557
C  PROGRAMMER:  G. I. KERLEY, T-4.                                      SESAME     558
C                                                                       SESAME     559
C  DATE:        18 JULY 1979                                            SESAME     560
C                                                                       SESAME     561
C-----------------------------------------------------------------------SESAME     562
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM        2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM        3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM        4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                        PARAM        5
      LEVEL 2,TBLS                                                      SESAME     564
      DIMENSION YY(6)                                                   SESAME     565
      COMMON/SESDAT/TBLS(NSD)                                           SESAME     566
      COMMON/INTORD/IFN                                                 SESAME     567
      COMMON/RTBLK1/LOCX,KX,LOCY,KY,I,N,IP,X,Y(2)                       SESAME     568
      IF(IFN.EQ.1) GO TO 6                                              SESAME     569
      IF(IP.EQ.0) GO TO 3                                               SESAME     570
C  CALCULATE COEFFICIENTS FOR RATIONAL FUNCTION INTERPOLATION            SESAME     571
      IX = LOCX+KX*(I-1)                                                SESAME     572
      IY = LOCY+KY*(I-1)                                                SESAME     573
      YY(3) = TBLS(IX)                                                  SESAME     574
      YY(4) = TBLS(IX+KX)-YY(3)                                         SESAME     575
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      YY(1) = TBLS(IY)                                                          SESAME    576
      YY(2) = (TBLS(IY+KY)-YY(1))/YY(4)                                         SESAME    577
      IF(I.EQ.N-1) GO TO 1                                                      SESAME    578
      SP = (TBLS(IY+KY+KY)-TBLS(IY+KY))/(TBLS(IX+KX+KX)-TBLS(IX+KX))            SESAME    579
      YY(6) = (SP-YY(2))/(TBLS(IX+KX+KX)-YY(3))                                 SESAME    580
      IF(I.GT.1) GO TO 1                                                        SESAME    581
      IF(YY(2)*(YY(2)-YY(4)*YY(6)).LE.0.) YY(6)=YY(2)/YY(4)                     SESAME    582
      YY(5) = YY(6)                                                             SESAME    583
      GO TO 2                                                                   SESAME    584
 1    DM = YY(3)-TBLS(IX-KX)                                                    SESAME    585
      SM = (YY(1)-TBLS(IY-KY))/DM                                               SESAME    586
      YY(5) = (YY(2)-SM)/(YY(4)+DM)                                             SESAME    587
      IF(I.EQ.N-1) YY(6)=YY(5)                                                  SESAME    588
      IF(I.GT.2) GO TO 2                                                        SESAME    589
      IF(SM*(SM-DM*YY(5)).LE.0.) YY(5)=(YY(2)-SM-SM)/YY(4)                      SESAME    590
 2    IF(YY(6).NE.0.) YY(5)=YY(5)/YY(6)                                         SESAME    591
C  EVALUATE RATIONAL FUNCTION FROM PRECALCULATED COEFFICIENTS                   SESAME    592
 3    Q = X-YY(3)                                                               SESAME    593
      R = YY(4)-Q                                                               SESAME    594
      IF(R.NE.0.) GO TO 4                                                       SESAME    595
      W = 1.                                                                    SESAME    596
      GO TO 5                                                                   SESAME    597
 4    W = 1.-1./(1.+ABS(YY(5)*Q/R))                                             SESAME    598
 5    F = YY(6)*(W+YY(5)*(1.-W))                                                SESAME    599
      Y(1) = YY(1)+Q*(YY(2)-R*F)                                                SESAME    600
      Y(2) = YY(2)+(Q-R)*F+YY(4)*W*(F-YY(6))                                    SESAME    601
      RETURN                                                                    SESAME    602
C  CALCULATE COEFFICIENTS FOR LINEAR INTERPOLATION                              SESAME    603
 6    IF(IP.EQ.0) GO TO 7                                                       SESAME    604
      IX = LOCX+KX*(I-1)                                                        SESAME    605
      IY = LOCY+KY*(I-1)                                                        SESAME    606
      YY(3) = TBLS(IX)                                                          SESAME    607
      YY(1) = TBLS(IY)                                                          SESAME    608
      YY(2) = (TBLS(IY+KY)-YY(1))/(TBLS(IX+KX)-YY(3))                           SESAME    609
C  CALCULATE LINEAR ESTIMATE FROM PRECALCULATED COEFFICIENTS                    SESAME    610
 7    Y(1) = YY(1)+YY(2)*(X-YY(3))                                              SESAME    611
      Y(2) = YY(2)                                                              SESAME    612
      RETURN                                                                    SESAME    613
      END                                                                       SESAME    614
```

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      SUBROUTINE T4DATI                                                 SESAME    615
C-----------------------------------------------------------------------SESAME    616
C                                                                       SESAME    617
C  SUBROUTINE:  T4DATI                                                  SESAME    618
C                                                                       SESAME    619
C  PURPOSE:     SEARCH/INTERPOLATE FOR PRESSURE AND TEMPERATURE         SESAME    620
C               AS FUNCTIONS OF REGION, DENSITY AND ENERGY,             SESAME    621
C               USING PACKED SESAME 2 DATA STRING OF TYPE 302           SESAME    622
C                                                                       SESAME    623
C               COMMON/SESIN/IR,IDT,R,E,IBR,IFL                         SESAME    624
C               COMMON/SESOUT/P(3),T(3)                                 SESAME    625
C               IR    (INPUT) - MATERIAL REGION  NUMBER                 SESAME    626
C               IDT   (INPUT) - DATA TYPE INDICATOR                     SESAME    627
C               R     (INPUT) - DENSITY                                 SESAME    628
C               E     (INPUT) - INTERNAL ENERGY                         SESAME    629
C               P,T (OUTPUT) - PRESSURE, TEMPERATURE VECTORS            SESAME    630
C                 P(1),T(1) = PRESSURE AND TEMPERATURE                  SESAME    631
C                 P(2),T(2) = DENSITY DERIVATIVES                       SESAME    632
C                 P(3),T(3) = ENERGY DERIVATIVES                        SESAME    633
C               IBR   (INPUT) - 0=COMPUTE BOTH P AND T                  SESAME    634
C                               1=COMPUTE P ONLY                        SESAME    635
C                               2=COMPUTE T ONLY                        SESAME    636
C               COMMON/SESDAT/TBLS                                      SESAME    637
C               TBLS (INPUT) - TABLE STORAGE ARRAY                      SESAME    638
C                                                                       SESAME    639
C  REMARKS:     ADAPTED FROM T-4 SESAME 2 ROUTINES S2EOSI AND           SESAME    640
C               LA302A.  PRESSURE AND TEMPERATURE ARE PACKED.           SESAME    641
C               THE SEARCH INDICES AND INTERPOLATION CONSTANTS          SESAME    642
C               ARE SAVED AND REUSED, IF POSSIBLE.                      SESAME    643
C                                                                       SESAME    644
C       *****   SYSTEM DEPENDENT FEATURE.  THE CONSTANT NSFT            SESAME    645
C       *****   IN STATEMENT 60 SHOULD BE SET TO 1/2 THE BIT            SESAME    646
C       *****   LENGTH.  FOR A CDC 7600, NSFT = 30.                     SESAME    647
C                                                                       SESAME    648
C  EXTERNALS:   RATFN1 (1-D INTERPOLATION ROUTINE)                      SESAME    649
C               T4INTP (2-D INTERPOLATION ROUTINE)                      SESAME    650
C                                                                       SESAME    651
C  PROGRAMMER:  G. I. KERLEY AND B. I. BENNETT, T-4.                    SESAME    652
C               J. ABDALLAH,JR.                                         SESAME    653
C                                                                       SESAME    654
C  DATE:        2 AUGUST 1978                                           SESAME    655
C                                                                       SESAME    656
C-----------------------------------------------------------------------SESAME    657
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM       2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM       3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM       4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                        PARAM       5
      LEVEL 2,TBLS                                                     SESAME    659
      COMMON/S2DIR/LCMX,NREG,LCFW(ML,1)                                SESAME    660
      COMMON/RTBLK1/LOCR,KX,LOCE,KY,IRX,N,ISAME,RX1,PX1(2)             SESAME    661
      COMMON/RTBLK2/LOCX,IX,NX,LOCY,IY,NY,LOCZ,NZ,NSFT,                SESAME    662
     $ RX2,ET,PX2(3),INT,IDS,ZZ(32)                                    SESAME    663
      COMMON/SESIN/IR,IDT,R,E,IBR,IFL                                  SESAME    664
      COMMON/SESOUT/P(3),T(3)                                          SESAME    665
      COMMON/SESDAT/TBLS(NSD)                                          SESAME    666
      DATA LOCLST,IP,IT/0,1,1/                                         SESAME    667
C  LOC IS POINTER TO START OF DATA STRING FOR REGION IR                 SESAME    668
      LOC = LCFW(IR,IDT)+2                                             SESAME    669
C  TEST TO SEE IF THE MATERIAL IS THE SAME AS LAST CALL                 SESAME    670
      IF(LOC.EQ.LOCLST) GO TO 5                                        SESAME    671
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C  THE FOLLOWING OPERATIONS DO NOT NEED TO BE REPEATED                SESAME   672
      NX = TBLS(LOC)                                                  SESAME   673
      NY = TBLS(LOC+1)                                                SESAME   674
      N = NX                                                          SESAME   675
      LOCR = LOC+2                                                    SESAME   676
      KX = 1                                                          SESAME   677
      LOCX = LOCR                                                     SESAME   678
      LOCY = LOCX+NX                                                  SESAME   679
      LOCE = LOCY+NY                                                  SESAME   680
      KY = 1                                                          SESAME   681
      LOCZ = LOCE+NX                                                  SESAME   682
      NZ = 1                                                          SESAME   683
C  UNLESS A NEW REGION HAS BEEN ENTERED                               SESAME   684
      LOCLST=LOC                                                      SESAME   685
      IXLAST = 0                                                      SESAME   686
      IYLAST = 0                                                      SESAME   687
      LOCI = LOCX+NX/2-1                                              SESAME   688
      LOCJ = LOCY+NY/2-1                                              SESAME   689
      LOCNX=LOCX+NX-2                                                 SESAME   690
      LOCNY=LOCY+NY-2                                                 SESAME   691
C  SEARCH FOR DENSITY INDEX                                           SESAME   692
 5    IF(R.LT.TBLS(LOCI)) GO TO 15                                    SESAME   693
 10   IF(R.LT.TBLS(LOCI+1)) GO TO 20                                  SESAME   694
      IF(LOCI.EQ.LOCNX) GO TO 20                                      SESAME   695
      LOCI=LOCI+1                                                     SESAME   696
      GO TO 10                                                        SESAME   697
 15   IF(LOCI.EQ.LOCX) GO TO 20                                       SESAME   698
      LOCI=LOCI-1                                                     SESAME   699
      IF(R.LT.TBLS(LOCI)) GO TO 15                                    SESAME   700
 20   IX=LOCI-LOCX+1                                                  SESAME   701
C  INTERPOLATE FOR ENERGY ON COLD CURVE.  IF ISAME = 0, DENSITY       SESAME   702
C  INDEX IS THE SAME AS IN THE LAST CALL TO THIS ROUTINE              SESAME   703
      IRX = IX                                                        SESAME   704
      ISAME = IABS(IX-IXLAST)                                         SESAME   705
      RX1=R                                                           SESAME   706
      CALL RATFN1                                                     SESAME   707
      ET = AMAX1(0.,E-PX1(1))                                         SESAME   708
      DECDR = PX1(2)                                                  SESAME   709
      RX2=R                                                           SESAME   710
C  SEARCH FOR ENERGY INDEX                                            SESAME   711
      IF(ET.LT.TBLS(LOCJ)) GO TO 35                                   SESAME   712
 30   IF(ET.LT.TBLS(LOCJ+1)) GO TO 40                                 SESAME   713
      IF(LOCJ.EQ.LOCNY) GO TO 40                                      SESAME   714
      LOCJ=LOCJ+1                                                     SESAME   715
      GO TO 30                                                        SESAME   716
 35   IF(LOCJ.EQ.LOCY) GO TO 40                                       SESAME   717
      LOCJ=LOCJ-1                                                     SESAME   718
      IF(ET.LT.TBLS(LOCJ)) GO TO 35                                   SESAME   719
 40   IY=LOCJ-LOCY+1                                                  SESAME   720
C  IF ISAME = 0,  DENSITY AND TEMPERATURE INDICES ARE                 SESAME   721
C  THE SAME AS IN THE LAST CALL TO THIS ROUTINE                       SESAME   722
      ISAME = ISAME+IABS(IY-IYLAST)                                   SESAME   723
      IP = MIN0(1,IP+ISAME)                                           SESAME   724
      IT = MIN0(1,IT+ISAME)                                           SESAME   725
      IXLAST = IX                                                     SESAME   726
      IYLAST = IY                                                     SESAME   727
      IDS=(IDT-1)*32+1                                                SESAME   728
      IF(IBR.EQ.2) GO TO 50                                           SESAME   729
C  PRESSURE CALCULATION                                               SESAME   730
      NSFT = 0                                                        SESAME   731
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      INT=IP                                                            SESAME    732
      CALL T4INTP                                                       SESAME    733
      P(1)=PX2(1)                                                       SESAME    734
      P(2)=PX2(2)-DECDR*PX2(3)                                          SESAME    735
      P(3)=PX2(3)                                                       SESAME    736
      IP = 0                                                            SESAME    737
      IF(IBR.EQ.1) RETURN                                               SESAME    738
C  TEMPERATURE CALCULATION                                              SESAME    739
 50   NSFT = 30                                                         SESAME    740
      INT=IT                                                            SESAME    741
      IDS=IDS+16                                                        SESAME    742
      CALL T4INTP                                                       SESAME    743
      T(1)=PX2(1)                                                       SESAME    744
      T(2)=PX2(2)-DECDR*PX2(3)                                          SESAME    745
      T(3)=PX2(3)                                                       SESAME    746
      IT = 0                                                            SESAME    747
      RETURN                                                            SESAME    748
      END                                                               SESAME    749
```

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      SUBROUTINE T4RTPE(IR,IDT,TBLS,R,T,P,E,IFL)                        SESAME    750
C-----------------------------------------------------------------------SESAME    751
C                                                                       SESAME    752
C  SUBROUTINE T4RTPE(IR,IDT,TBLS,R,T,P,E,IFL)                           SESAME    753
C                                                                       SESAME    754
C  PURPOSE    TO FIND PRESSURE AND ENERGY AS FUNCTIONS                  SESAME    755
C             OF DENSITY AND TEMPERATURE FROM A                         SESAME    756
C             SESAME TYPE 302 TABLE USING NEWTONS METHOD.               SESAME    757
C                                                                       SESAME    758
C  ARGUMENTS  IR         (INPUT)   REGION NO.                          SESAME    759
C             IDT        (INPUT)   DATA TYPE FOR 302 TABLES            SESAME    760
C             TBLS       (INPUT)   TABLE STORAGE ARRAY                 SESAME    761
C             T          (INPUT)   TEMPERATURE                         SESAME    762
C             P          (OUTPUT)  PRESSURE                            SESAME    763
C             E          (OUTPUT)  ENERGY                              SESAME    764
C             IFL        (OUTPUT)  OUTPUT FLAG                         SESAME    765
C                                  =1 FOR SUCCESS                     SESAME    766
C                                  =0 FOR FAILURE                     SESAME    767
C                                                                       SESAME    768
C  REMARKS     NONE                                                     SESAME    769
C                                                                       SESAME    770
C  EXTERNALS   T4EOSA                                                   SESAME    771
C                                                                       SESAME    772
C  PROGRAMMER  J.ABDALLAH,JR.                                           SESAME    773
C                                                                       SESAME    774
C  DATE        5 JULY 1979                                              SESAME    775
C                                                                       SESAME    776
C-----------------------------------------------------------------------SESAME    777
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM       2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM       3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM       4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                        PARAM       5
      LEVEL 2,TBLS                                                     SESAME    779
      COMMON/S2DIR/LCMX,NREG,LCFW(ML,1)                                SESAME    780
      DIMENSION TBLS(1)                                                SESAME    781
      COMMON/SESIN/IRXX,IDTX,RX,EX,IBR,IFLX                            SESAME    782
      COMMON/SESOUT/ZP(3),ZT(3)                                        SESAME    783
      IBR=0                                                            SESAME    784
      IFLX=1                                                           SESAME    785
      RX=R                                                             SESAME    786
      IRXX=IR                                                          SESAME    787
      IDTX=IDT                                                         SESAME    788
      LOC=LCFW(IR,IDT)                                                 SESAME    789
      NR=TBLS(LOC+2)                                                   SESAME    790
      NE=TBLS(LOC+3)                                                   SESAME    791
C . . GET INITIAL GUESS ON ENERGY                                      SESAME    792
C . . FIND CLOSEST DENSITY INDEX                                       SESAME    793
      LOCX=LOC+4                                                       SESAME    794
      IXR=1                                                            SESAME    795
      DELS=ABS(R-TBLS(LOCX))                                           SESAME    796
      IF(NR.EQ.1) GO TO 20                                             SESAME    797
      DO 10 J=2,NR                                                     SESAME    798
      LOCX=LOCX+1                                                      SESAME    799
      DEL=ABS(R-TBLS(LOCX))                                            SESAME    800
      IF(DEL.GT.DELS) GO TO 10                                         SESAME    801
      IRX=J                                                            SESAME    802
      DELS=DEL                                                         SESAME    803
 10   CONTINUE                                                         SESAME    804
C . . FIND THE ENERGY INDEX ASSOCIATED WITH THE CLOSEST TEMP           SESAME    805
 20   LOCX=LOC+3+NR+NE+NR+IRX                                          SESAME    806
```

```
      DELS=TBLS(LOCX)                                                   SESAME    807
      DELS=SHIFT(DELS,30)                                               SESAME    808
      DELS=ABS(T-DELS)                                                  SESAME    809
      IEX=1                                                             SESAME    810
      IF(NE.EQ.1) GO TO 40                                              SESAME    811
      DO 30 J=2,NE                                                      SESAME    812
      LOCX=LOCX+NR                                                      SESAME    813
      DEL=TBLS(LOCX)                                                    SESAME    814
      DEL=SHIFT(DEL,30)                                                 SESAME    815
      DEL=ABS(T-DEL)                                                    SESAME    816
      IF(DEL.GT.DELS) GO TO 30                                          SESAME    817
      IEX=J                                                             SESAME    818
      DELS=DEL                                                          SESAME    819
 30   CONTINUE                                                          SESAME    820
C . . INITIAL GUESS ON ENERGY                                           SESAME    821
 40   EX=TBLS(LOC+3+NR+IEX)+TBLS(LOC+3+NR+NE+IRX)                       SESAME    822
C . . ITERATE USING NEWTONS METHOD                                      SESAME    823
      K=0                                                               SESAME    824
      IFL=1                                                             SESAME    825
 50   K=K+1                                                             SESAME    826
      IF(K.EQ.50) GO TO 90                                              SESAME    827
      CALL T4EOSA                                                       SESAME    828
      E=EX                                                              SESAME    829
      P=ZP(1)                                                           SESAME    830
      TTEST=ABS(T-ZT(1))-1.0E-05*(ABS(T)+1.0E-02)                       SESAME    831
      IF(TTEST.LT.0.) RETURN                                            SESAME    832
      D=-ZT(3)                                                          SESAME    833
      IF(D.EQ.C.0) GO TO 90                                             SESAME    834
      EX=EX-(T-ZT(1))/D                                                 SESAME    835
      GO TO 50                                                          SESAME    836
 90   IFL=0                                                             SESAME    837
      RETURN                                                            SESAME    838
      END                                                               SESAME    839
```

```
      SUBROUTINE INV301(DSTR,LOC,RO,LDS)                                SESAME    840
C-----------------------------------------------------------------------SESAME    841
C                                                                       SESAME    842
C  SUBROUTINE:  INV301(DSTR,LOC,RO,LDS)                                 SESAME    843
C                                                                       SESAME    844
C  PURPOSE:     INVERT DATA STRING OF TYPE 301 TO TYPE 302.             SESAME    845
C                                                                       SESAME    846
C  ARGUMENTS:   DSTR (INPUT) - TABLE STORAGE ARRAY                      SESAME    847
C               LOC  (INPUT) - STARTING LOCATION OF DATA STRING         SESAME    848
C                              IN DSTR                                  SESAME    849
C               RO   (INPUT) - APPROXIMATE DENSITY OF SOLID             SESAME    850
C               LDS (OUTPUT) - LENGTH OF NEW DATA STRING                SESAME    851
C                                                                       SESAME    852
C  REMARKS:     DSTR CAN BE DECLARED LCM ON THE CDC 7600.               SESAME    853
C               THIS ROUTINE OVERWRITES LOCATIONS FOLLOWING THE         SESAME    854
C               DATA STRING.  IT EXPANDS THE STRING BY NR WORDS,        SESAME    855
C               WHERE NR IS THE NUMBER OF DENSITIES.  IT ALSO           SESAME    856
C               USES 3*NT WORDS AS TEMPORARY STORAGE, WHERE NT          SESAME    857
C               IS THE NUMBER OF TEMPERATURES.                          SESAME    858
C                                                                       SESAME    859
C  EXTERNALS:   ISRCHK, RATFN1.                                         SESAME    860
C                                                                       SESAME    861
C  PROGRAMMER:  G. I. KERLEY, T-4.                                      SESAME    862
C                                                                       SESAME    863
C  DATE:        4 OCTOBER 1977                                          SESAME    864
C                                                                       SESAME    865
C-----------------------------------------------------------------------SESAME    866
      LEVEL 2,DSTR                                                      SESAME    867
      DIMENSION DSTR(1)                                                 SESAME    868
      COMMON/INTORD/IFN                                                 SESAME    869
      COMMON/RTBLK1/LOCX,NR,LOCY,KY,JX,NT,INT,ET,Z(2)                   SESAME    870
      INT=1                                                             SESAME    871
      IFNS=IFN                                                          SESAME    872
      IFN=0                                                             SESAME    873
      NR = DSTR(LOC)                                                    SESAME    874
      NT = DSTR(LOC+1)                                                  SESAME    875
      LOCT = 2+NR+LOC                                                   SESAME    876
      LCEC = LOCT+NT                                                    SESAME    877
      LOCP = LCEC+NR                                                    SESAME    878
      LOCE = LOCP+NR*NT                                                 SESAME    879
      LOCN = LOCE+NR*NT                                                 SESAME    880
      IMAX = 2*NR*NT                                                    SESAME    881
      DO 1 I=1,IMAX                                                     SESAME    882
 1    DSTR(LOCN-I) = DSTR(LOCN-I-NR)                                    SESAME    883
      DO 2 I=1,NR                                                       SESAME    884
      JJ = LOCE+I-1                                                     SESAME    885
      Q = 1.E-12*ABS(DSTR(JJ))                                          SESAME    886
      DSTR(LCEC+I-1) = DSTR(JJ)                                         SESAME    887
      DSTR(JJ) = 0.                                                     SESAME    888
      DO 2 J=2,NT                                                       SESAME    889
      JJ = JJ+NR                                                        SESAME    890
      DSTR(JJ) = DSTR(JJ)-DSTR(LCEC+I-1)                                SESAME    891
      IF(DSTR(JJ)-DSTR(JJ-NR).LT.Q) DSTR(JJ)=DSTR(JJ-NR)+Q              SESAME    892
 2    CONTINUE                                                          SESAME    893
      I = ISRCHK(RO,DSTR(LOC+3),NR-2,1,0)+1                             SESAME    894
      DO 3 J=1,NT                                                       SESAME    895
      DSTR(LOCN+J-1) = DSTR(LOCT+J-1)                                   SESAME    896
 3    DSTR(LOCT+J-1) = DSTR(LOCE+I-1+NR*(J-1))                          SESAME    897
      DO 5 I=1,NR                                                       SESAME    898
      LOCX = LOCE+I-1                                                   SESAME    899
```

```
      DO 4 J=1,NT                                                        SESAME    900
      ET = DSTR(LOCT+J-1)                                                SESAME    901
      JX = ISRCHK(ET,DSTR(LOCX+NR),NT-2,NR,0)+1                          SESAME    902
      LOCY = LOCP+I-1                                                    SESAME    903
      KY = NR                                                            SESAME    904
      CALL RATFN1                                                        SESAME    905
      DSTR(LOCN+NT+J-1) = Z(1)                                           SESAME    906
      LOCY = LOCN                                                        SESAME    907
      KY = 1                                                             SESAME    908
      CALL RATFN1                                                        SESAME    909
4     DSTR(LOCN+NT+NT+J-1) = Z(1)                                        SESAME    910
      DO 5 J=1,NT                                                        SESAME    911
      DSTR(LOCP+I-1+NR*(J-1)) = DSTR(LOCN+NT+J-1)                        SESAME    912
5     DSTR(LOCX+NR*(J-1)) = DSTR(LOCN+NT+NT+J-1)                         SESAME    913
      LDS = LOCN-LOC                                                     SESAME    914
      IFN=IFNS                                                           SESAME    915
      RETURN                                                             SESAME    916
      END                                                                SESAME    917
```

```
      SUBROUTINE T4EOSA                                                 SESAME    918
C-----------------------------------------------------------------------SESAME    919
C                                                                       SESAME    920
C  SUBROUTINE  T4EOSA                                                   SESAME    921
C                                                                       SESAME    922
C  PURPOSE     TO COMPUTE A DENSITY SCALED,ENERGY SHIFTED,              SESAME    923
C              EQUATION OF STATE AUGMENTED BY A ANALYTIC                SESAME    924
C              PRESSURE RAMP                                            SESAME    925
C                                                                       SESAME    926
C              COMMON/SESIN/IR,IDT,R,E,IBR,IFL                          SESAME    927
C              COMMON/SESOUT/P(3),T(3)                                  SESAME    928
C              IR    (INPUT)   REGION. NO.                              SESAME    929
C              IDT   (INPUT)   DATA TYPE CORRESPONDING TO ENERGY BASED  SESAME    930
C                              (TYPE 302) SESAME TABLE                  SESAME    931
C              R     (INPUT)   DENSITY                                  SESAME    932
C              E     (INPUT)   INTERNAL ENERGY                          SESAME    933
C              P(1)  (OUTPUT)  PRESSURE                                 SESAME    934
C              P(2)  (OUTPUT)  DENSITY DERIVATIVE OF PRESSURE           SESAME    935
C              P(3)  (OUTPUT)  ENERGY DERIVATIVE OF PRESSURE            SESAME    936
C              T(1)  (OUTPUT)  TEMPERATURE                              SESAME    937
C              T(2)  (OUTPUT)  DENSITY DERIVATIVE OF TEMP               SESAME    938
C              T(3)  (OUTPUT)  ENERGY DERIVATIVE OF TEMP                SESAME    939
C              IBR   (INPUT)   =0 TO OUTPUT BOTH P AND T                SESAME    940
C                              =1 TO OUTPUT P ONLY                      SESAME    941
C                              =2 TO OUTPUT T ONLY                      SESAME    942
C              IFL   (IN/OUT)  INPUT                                    SESAME    943
C                              0=CHOOSE BETWEEN RAMP AND TABLES         SESAME    944
C                              1=FORCE USE OF TABLES                    SESAME    945
C                              OUTPUT                                   SESAME    946
C                              0=PRESSURE COMPUTED FROM RAMP            SESAME    947
C                              1=PPESSURE COMPUTED FROM TABLES          SESAME    948
C                              NOTE THAT THIS FLAG CAN BE USED          SESAME    949
C                              TO SATISFY REVERSIBILITY CONDITIONS.     SESAME    950
C                                                                       SESAME    951
C  REMARKS     COMMON/EOSCOM/ MUST BE SUPPLIED BY THE USER              SESAME    952
C              PROGRAM. NREG IS THE NUMBER OF REGIONS. THE ARRAYS       SESAME    953
C              CONTAIN VALUES FOR PARAMETERS IN EACH REGION,THEY ARE    SESAME    954
C              SR(IR) - DENSITY SCALE FACTOR FOR REGION IR              SESAME    955
C              ES(IR) - ENERGY SHIFT                                    SESAME    956
C              RO(IR) - RHOO FOR MATERIAL                               SESAME    957
C              A1(IR) - RAMP PARAMETER IF 0 THEN NO RAMP                SESAME    958
C              A2(IR) - RAMP PARAMETER                                  SESAME    959
C              A3(IR) - RAMP PARAMETER                                  SESAME    960
C              EM(IR) - MELT ENERGY                                     SESAME    961
C                                                                       SESAME    962
C  EXTERNALS   T4DATI                                                   SESAME    963
C                                                                       SESAME    964
C  PROGRAMMER  J.ABDALLAH,JR.                                           SESAME    965
C                                                                       SESAME    966
C  DATE        14 JUNE 1979                                             SESAME    967
C                                                                       SESAME    968
C-----------------------------------------------------------------------SESAME    969
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM       2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM       3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM       4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                        PARAM       5
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO INIT        2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),IBRN(ML),PLAP(ML),DRO(ML), INIT      3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),QO(ML),TMLT(ML),TMC(ML)            INIT        4
      COMMON/EOSCOM/SR(ML),ES(ML),                                      SESAME    972
```

```
     $               A1(ML),A2(ML),A3(ML),EM(ML),IRV(ML)                SESAME     973
      COMMON/SESIN/IR,IDT,R,E,IBR,IFL                                   SESAME     974
      COMMON/SESOUT/P(3),T(3)                                           SESAME     975
      DIMENSION RO(ML)                                                  SESAME     976
      EQUIVALENCE(RO,ROW)                                               SESAME     977
C . . SCALE DENSITY                                                     SESAME     978
      RSAVE=R                                                           SESAME     979
      R=SR(IR)*R                                                        SESAME     980
C . . SHIFT AND SCALE ENERGY                                            SESAME     981
      ESAVE=E                                                           SESAME     982
      E=(ES(IR)+E)/SR(IR)                                               SESAME     983
C . . COMPUTE EOS FROM TABLES                                           SESAME     984
      CALL T4DATI                                                       SESAME     985
C . . IF FORCED TABLES - RETURN                                         SESAME     986
      IF(IFL.EQ.1) RETURN                                               SESAME     987
      IF(IBR.NE.2) GO TO 5                                              SESAME     988
C . . TEMP ONLY                                                         SESAME     989
      IFL=1                                                             SESAME     990
      RETURN                                                            SESAME     991
 5    IF(A1(IR).NE.0.0) GO TO 10                                        SESAME     992
C . . NO RAMP INPUT RETURN                                              SESAME     993
      IFL=1                                                             SESAME     994
      RETURN                                                            SESAME     995
 10   IF(ESAVE.LE.EM(IR)) GO TO 20                                      SESAME     996
C . . ENERGY IS GREATER THAN THE MELT ENERGY - RETURN                   SESAME     997
      IFL=1                                                             SESAME     998
      RETURN                                                            SESAME     999
C . . COMPUTE RAMP PRESSURE                                             SESAME    1000
 20   COMP=RSAVE/RO(IR)                                                 SESAME    1001
      P1=A1(IR)*(COMP-1.0)                                              SESAME    1002
      DPR1=A1(IR)/RO(IR)                                                SESAME    1003
      IF(A2(IR).LE.0.0) GO TO 25                                        SESAME    1004
      P2=A2(IR)*(COMP-A3(IR))                                           SESAME    1005
      DPR2=A2(IR)/RO(IR)                                                SESAME    1006
      IF(P1.LT.P2) GO TO 25                                             SESAME    1007
      P1=P2                                                             SESAME    1008
      DPR1=DPR2                                                         SESAME    1009
 25   IF(P1.LT.P(1)) GO TO 30                                           SESAME    1010
C . . RAMP USED FOR PRESSURE                                            SESAME    1011
      IFL=0                                                             SESAME    1012
      P(1)=P1                                                           SESAME    1013
      P(2)=DPR1                                                         SESAME    1014
      P(3)=0.0                                                          SESAME    1015
      RETURN                                                            SESAME    1016
C . . PRESSURE FROM TABLES                                              SESAME    1017
 30   IFL=1                                                             SESAME    1018
      RETURN                                                            SESAME    1019
      END                                                               SESAME    1020
```

```
      SUBROUTINE PERTC8(IR,TBLS,ZBAR,ABAR)                              SESAME   1021
C                                                                       SESAME   1022
C     ROUTINE TO PERTURB A 3G1-LIKE EOS TABLE BY MEANS OF A GAUSSIAN    SESAME   1023
C     BUMP ON THE ISOTHERMS.  ONE MAY ALSO INCLUDE A HARDNESS           SESAME   1024
C     FACTOR FOR THE PRESSURE AND ENERGIES.                             SESAME   1025
C                                                                       SESAME   1026
      LEVEL 2,TBLS                                                      SESAME   1027
      PARAMETER (MCL=500,ML=21,NGC=19,MLGC=NGC*ML,MLDWDT=20*ML,         PARAM       2
     +NUMV=10,MQL=((NUMV+1)/3+1)*MCL+100,NDW=20,NCF=8,                  PARAM       3
     +MXDUMP=30,NDX=2*MXDUMP+2,MTAB=1,NTAB=MTAB*3742                    PARAM       4
     +,NSM=4,NWPM=3728,NSD=NSM*NWPM+132,ML2=100)                        PARAM       5
      COMMON/INIT/DTO(ML),XMU(ML),YO(ML),XL(ML),XV(ML),NV(ML),VO(ML),PO INIT        2
     +(ML),TO(ML),ROW(ML),JMIN(ML2),JMAX(ML2),I8RN(ML),PLAP(ML),DRO(ML), INIT      3
     +MAT(ML),UO(ML),UT(ML),DTCF(ML),OO(ML),TMLT(ML),TMC(ML)            INIT        4
      COMMON/S2DIR/LCMX,NREG,LCFW(ML,1)                                 S2DIR       2
      COMMON/T4PERT/LPERT(5),ZETA(5),VLOW(5),VHI(5),HARD(5)             T4PERT      2
      DIMENSION RO(ML)                                                  SESAME   1032
      EQUIVALENCE (RO,ROW)                                              SESAME   1033
      DIMENSION TBLS(1)                                                 SESAME   1034
      RHOZRO = RO(IR)                                                   SESAME   1035
      IF(RHOZRO.EQ.0.0) RHOZRO = TBLS(2)                                SESAME   1036
C                                                                       SESAME   1037
C     DOES THIS EOS GET PERTURBED?                                      SESAME   1038
C                                                                       SESAME   1039
      IM = ABS(TBLS(1))                                                 SESAME   1040
      DO 200 LI=1,5                                                     SESAME   1041
      IF(IM.EQ.IABS(LPERT(LI))) GO TO 202                               SESAME   1042
  200 CONTINUE                                                          SESAME   1043
      GO TO 299                                                         SESAME   1044
  202 CONTINUE                                                          SESAME   1045
C                                                                       SESAME   1046
C     DO PERTURBATION -- PRELIMINARY STUFF                              SESAME   1047
C                                                                       SESAME   1048
      VINLOW = 1.0/VLOW(LI)                                             SESAME   1049
      VINHI = 1.0/VHI(LI)                                               SESAME   1050
      CEN = 0.5*(VINLOW + VINHI)                                        SESAME   1051
      SIG = 2.0/(VINLOW - VINHI)                                        SESAME   1052
      LCEP = TBLS(3)                                                    SESAME   1053
      LTEP = TBLS(4)                                                    SESAME   1054
      C1 = ZETA(LI)*ZBAR*(8.3144E-03)/ABAR                              SESAME   1055
C                                                                       SESAME   1056
C     FIND THE COMPRESSION JUST LESS THAN CEN                           SESAME   1057
C                                                                       SESAME   1058
      RHOCEN = RHOZRO*CEN                                               SESAME   1059
      DO 210 LCEN = 1,LCEP                                              SESAME   1060
      IF(TBLS(4+LCEN).GT.RHOCEN) GO TO 211                              SESAME   1061
  210 CONTINUE                                                          SESAME   1062
  211 LCEN = LCEN - 1                                                   SESAME   1063
C                                                                       SESAME   1064
C     FIRST COMPUTE BIAS FOR PRESSURE AND ENERGY LOOKUP IN TBLS         SESAME   1065
C                                                                       SESAME   1066
      NPRSK = 4 + LCEP + LTEP                                           SESAME   1067
      NERSK = NPRSK + LCEP*LTEP                                         SESAME   1068
      ICEN = NPRSK + LCEN + 7*LCEP                                      SESAME   1069
C                                                                       SESAME   1070
C     ORIGINAL PRESSURE AT OR NEAR CENTER OF GAUSSIAN                   SESAME   1071
C                                                                       SESAME   1072
      PCEN = TBLS(ICEN)                                                 SESAME   1073
C                                                                       SESAME   1074
C     FIND THE REGION THAT NEEDS MODIFYING                              SESAME   1075
```

```
C       LOWEST COMPRESSION INDEX = IPL                                  SESAME   1076
        RINHI = RHOZRO*VINHI                                            SESAME   1077
        DO 212 IPL=1,LCEP                                               SESAME   1078
        IF(TBLS(4+IPL).GT.RINHI) GO TO 214                              SESAME   1079
  212   CONTINUE                                                        SESAME   1080
  214   IPL = IPL - 1                                                   SESAME   1081
C                                                                       SESAME   1082
C       HIGHEST COMPRESSION INDEX = IPH                                 SESAME   1083
C                                                                       SESAME   1084
        RINLOW = RHOZRO*VINLOW                                          SESAME   1085
        DO 215 IPH=IPL,LCEP                                             SESAME   1086
        IF(TBLS(4+IPH).GE.RINLOW) GO TO 216                             SESAME   1087
  215   CONTINUE                                                        SESAME   1088
  216   CONTINUE                                                        SESAME   1089
C                                                                       SESAME   1090
C       TABLE REPLACEMENT WITH PERTURBED VALUES                         SESAME   1091
C                                                                       SESAME   1092
        DO 230 JP=IPL,IPH                                               SESAME   1093
C       THIS IS THE COMPRESSION LOOP                                    SESAME   1094
        RHO = TBLS(4+JP)                                                SESAME   1095
        ETA = RHO/RHOZRO                                                SESAME   1096
        F = EXP(-(SIG*(CEN-ETA))**2)                                    SESAME   1097
        DO 231 JT=1,LTEP                                                SESAME   1098
C       THIS IS THE TEMPERATURE LOOP                                    SESAME   1099
        T = TBLS(4+LCEP+JT)                                             SESAME   1100
C       IDEAL GAS SHAPED BY A GAUSSIAN                                  SESAME   1101
        PHAT = F*C1*RHO*T                                               SESAME   1102
        MSKIP = JP + (JT-1)*LCEP                                        SESAME   1103
        IPX = NPRSK + MSKIP                                             SESAME   1104
        IEX = NERSK + MSKIP                                             SESAME   1105
        TBLS(IPX) = HARD(LI)*TBLS(IPX) + PHAT                           SESAME   1106
        TBLS(IEX) = HARD(LI)*TBLS(IEX)                                  SESAME   1107
  231   CONTINUE                                                        SESAME   1108
  230   CONTINUE                                                        SESAME   1109
  299   CONTINUE                                                        SESAME   1110
        RETURN                                                          SESAME   1111
        END                                                             SESAME   1112
```

V. SAMPLE PROBLEMS

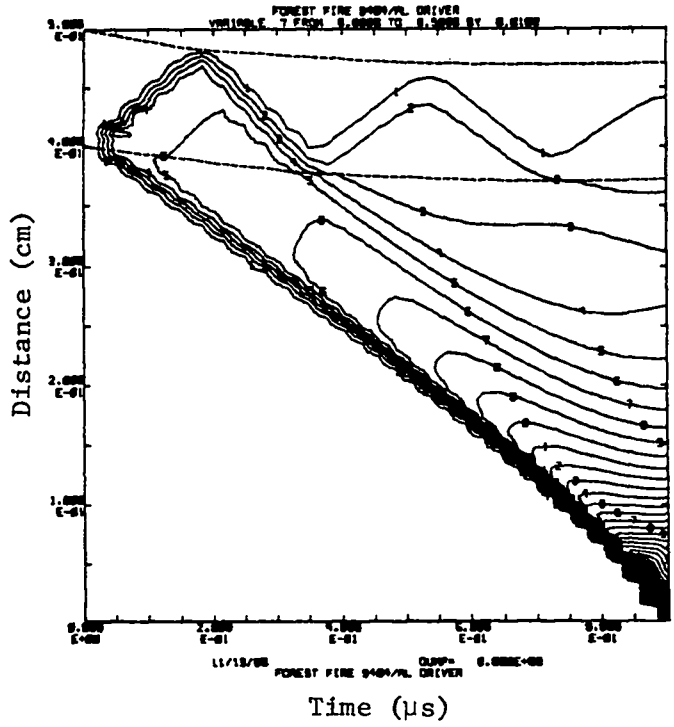
To aid users in setting up problems in HYDROX, we have included a set of sample problems. Each of the problems is concerned with the use of HE in contact with a metal plate. The first two sample problems consist of an aluminum plate striking a piece of PBX-9404 treated in the Forest Fire HE model. As shown in the results, the 1-mm-thick plate drives the PBX-9404 to a full detonation, whereas the 0.5-mm driven system does not proceed to full detonation. The third problem is a 3-cm piece of PBX-9404 treated in the buildup HE model driving an aluminum plate. Spall layers are allowed to form in the aluminum and are evident in the distance-time plot. The last problem consists of 5 cm of Comp B in contact with an aluminum plate.

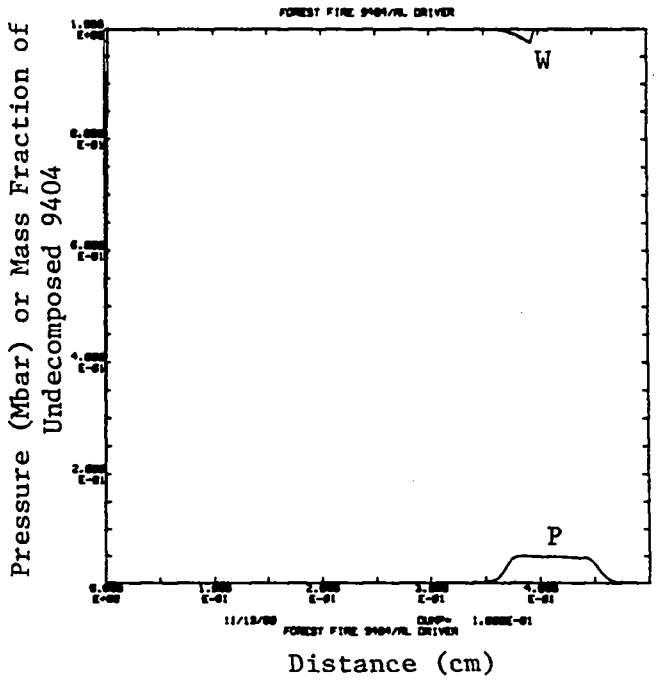
All plots were obtained by using the graphics code GAS, and for the distance-time plots the code OTGAS was used as an intermediate step. Further details on the graphics may be found in LASL Utility Routine LTSS-523.

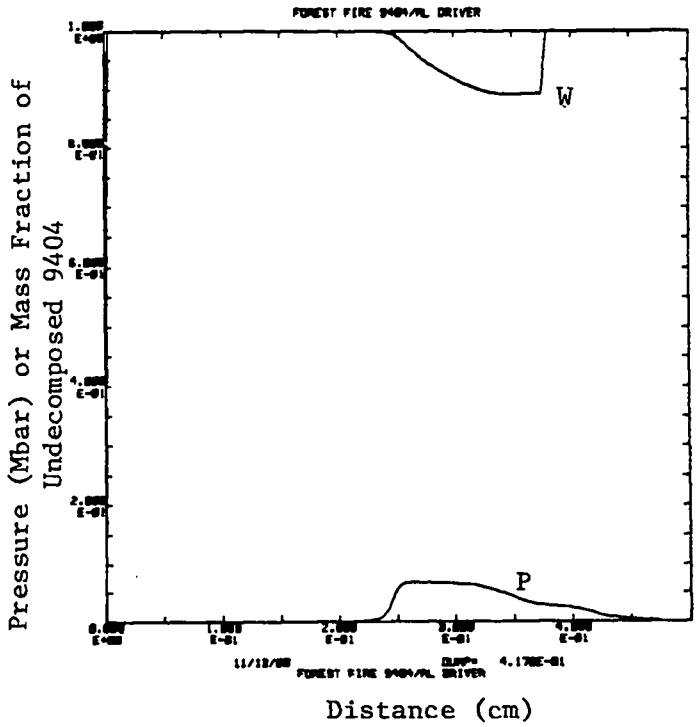
A. 1 mm of Aluminum Impacting PBX-9404 Using the Forest Fire Model

Input File DATA

```
P$INP NM=2,TEND=1.,NG=20,IALPH=1,R0=.5,
      NMAX=35,NADD=2,
      LABEL=27H FOREST FIRE 9404/AL DRIVER $
P$SU MAT=2,R2=.4,NCI=30,U0=-.1,ME=1 $
P$ESC NV=2,XV=.3 $
P$SU MAT=24,R2=0.,NCI=120 $
```







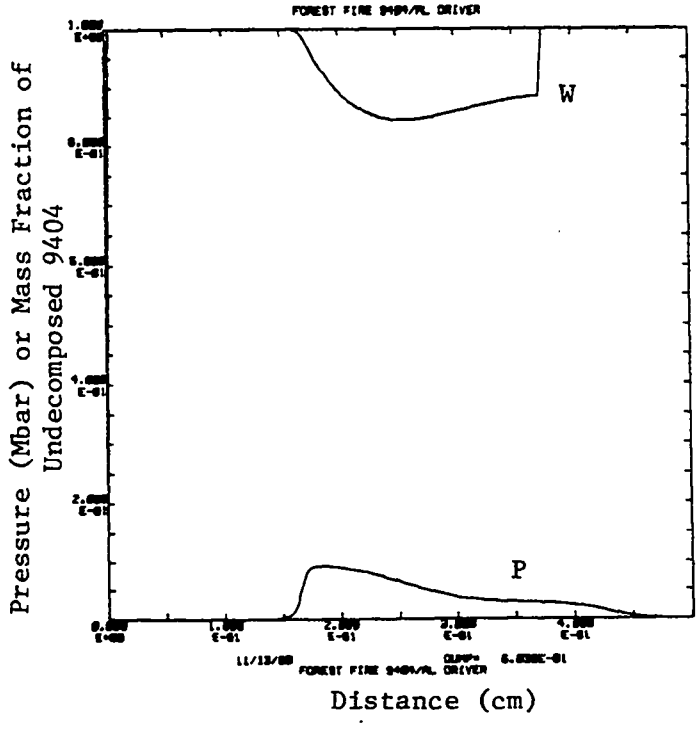
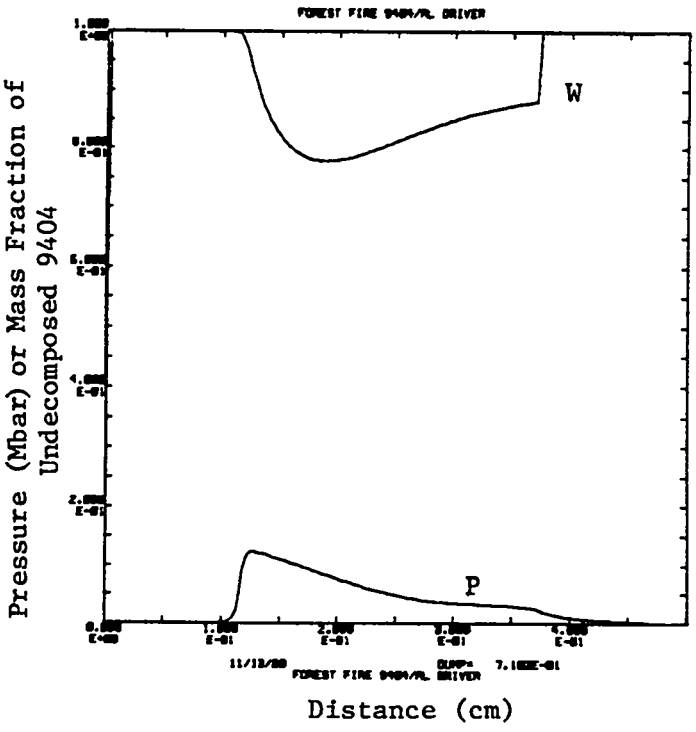
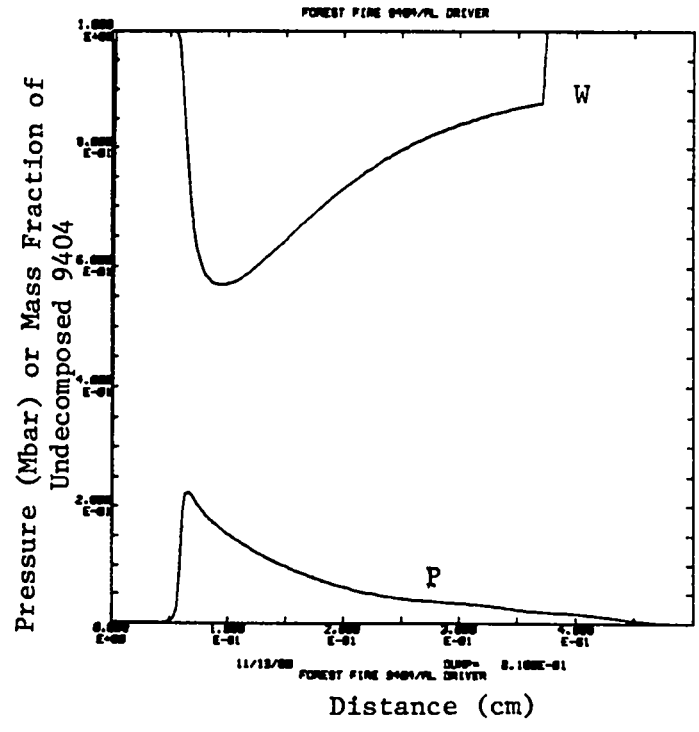


Fig. 9.
Pressure contours (0.010 Mbar).


Pressure (Mbar) or Mass Fraction of Undecomposed 9404
W
P
Distance (cm)


Pressure (Mbar) or Mass Fraction of Undecomposed 9404
W
P
Distance (cm)

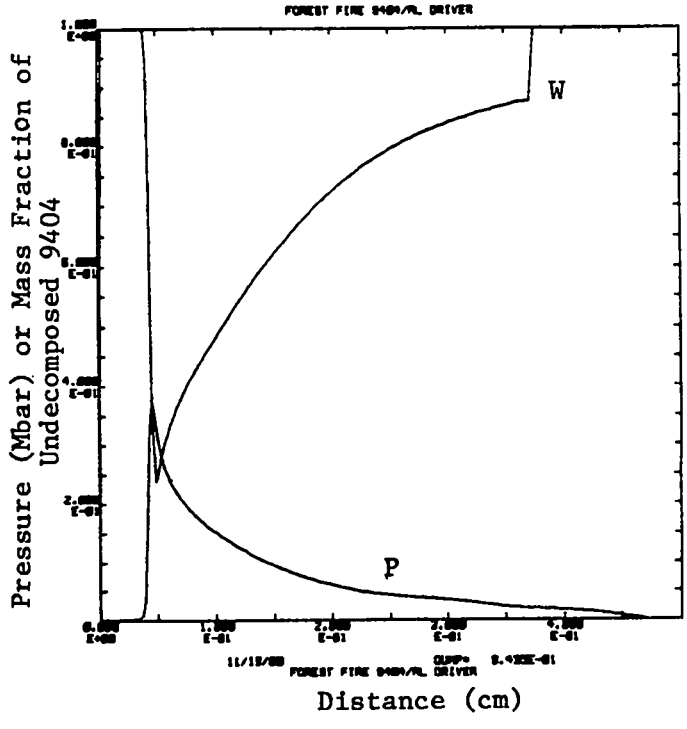

Pressure (Mbar) or Mass Fraction of Undecomposed 9404
W
P
Distance (cm)

Fig. 9. (cont)

B. 0.5 mm of Al Impacting 9404 Using the Forest Fire Model

Input File DATA

```
P$INP NM=2,TEND=1.,NG=20,IALPH=1,RO=.45,
      NMAX=35,NADD=2,
      LABEL=27H FOREST FIRE 9404/AL DRIVER $
P$SU MAT=2,R2=.4,NCI=15,UO=-.1,ME=1 $
P$ESC NV=2,XV=.3 $
P$SU MAT=24,R2=0.,NCI=120 $
```

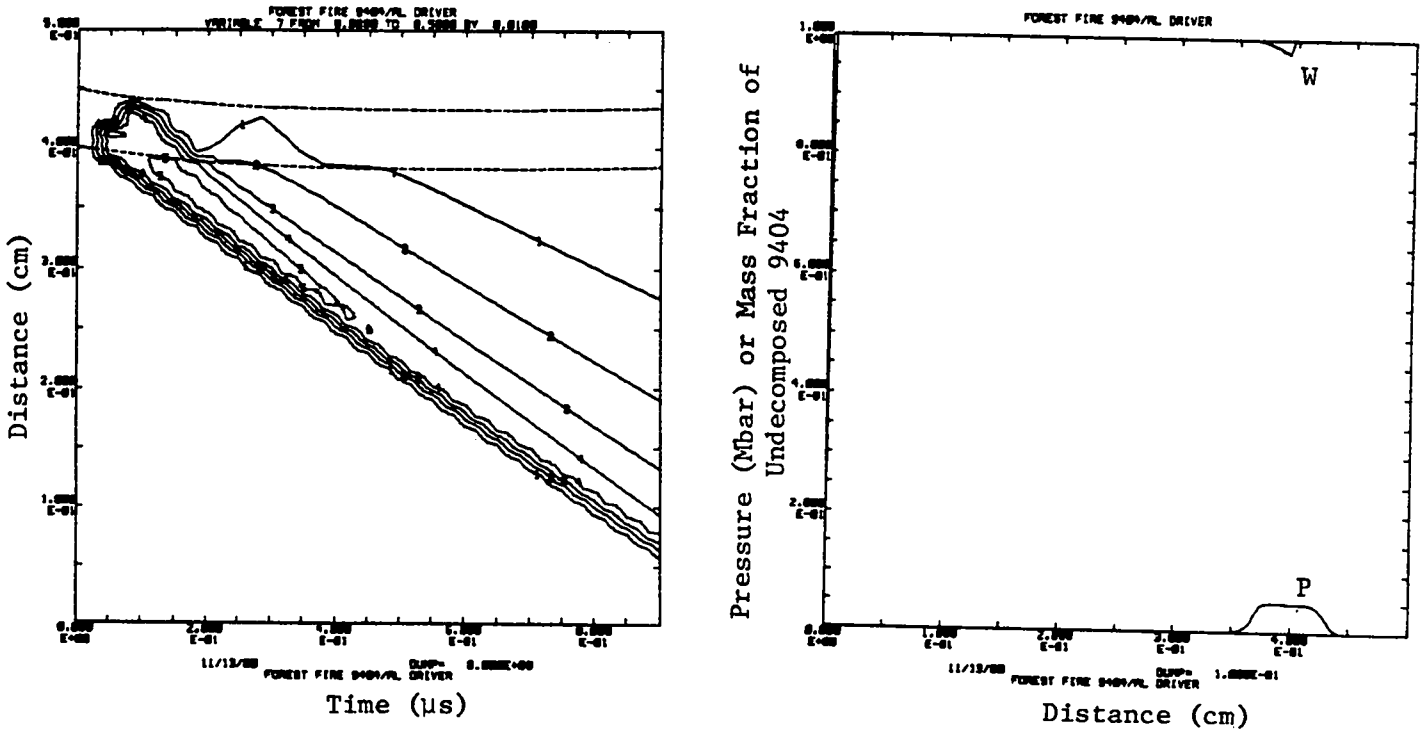
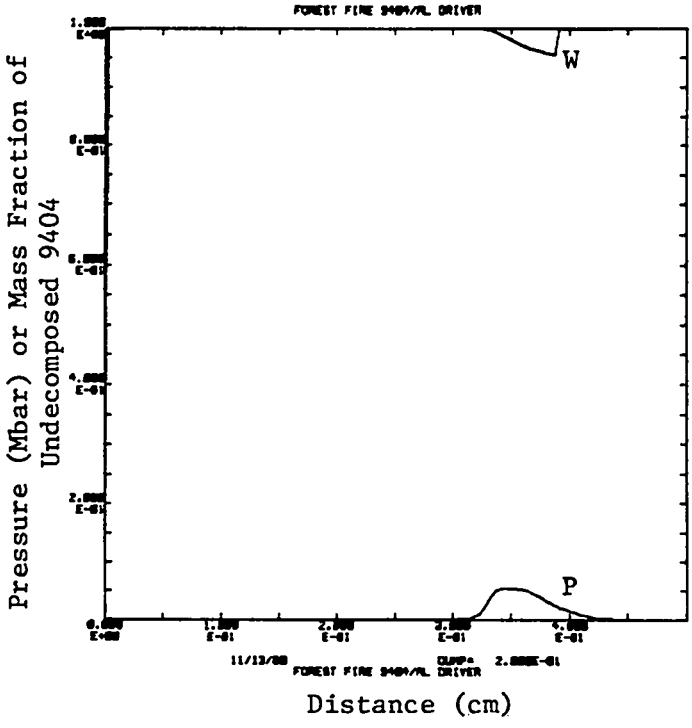
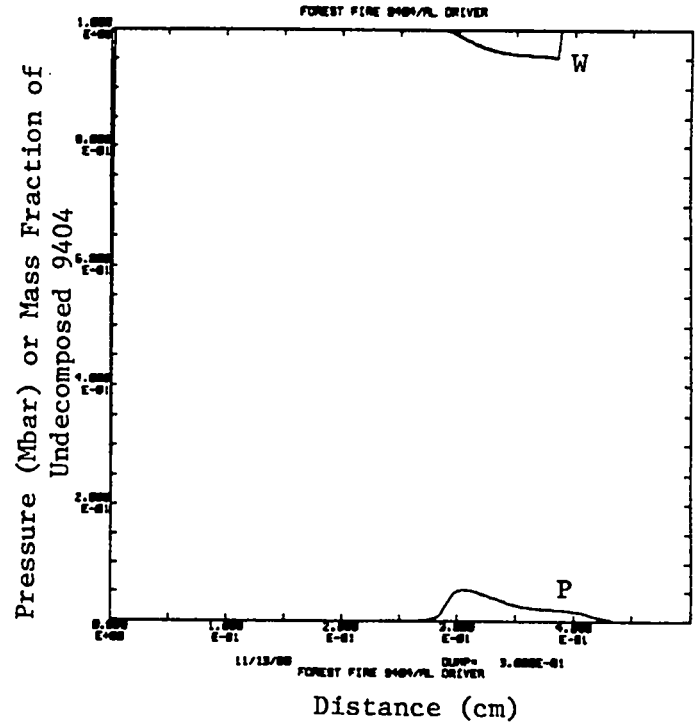


Fig. 10.
Pressure contours (0.010 Mbar)


FOREST FIRE 9404/RL DRIVER
W
P
Pressure (Mbar) or Mass Fraction of Undecomposed 9404
Distance (cm)


FOREST FIRE 9404/RL DRIVER
W
P
Pressure (Mbar) or Mass Fraction of Undecomposed 9404
Distance (cm)

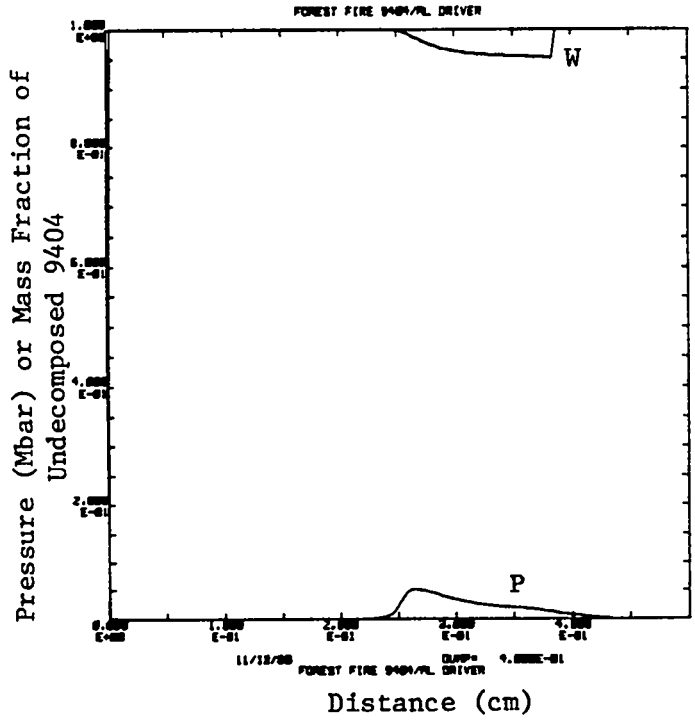
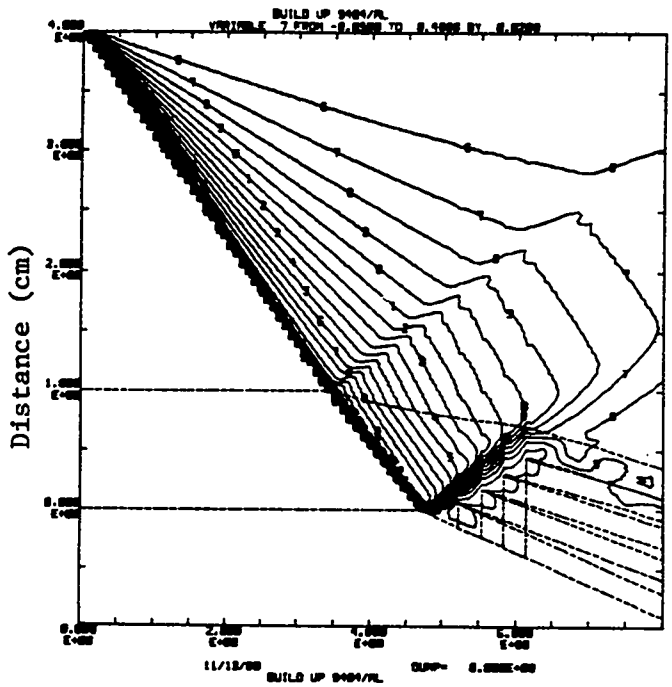

FOREST FIRE 9404/RL DRIVER
W
P
Pressure (Mbar) or Mass Fraction of Undecomposed 9404
Distance (cm)

Fig. 10. (cont)

C. 3 cm of 9404 in the Buildup Model Pushing 1 cm of Al

Input File DATA

```
P$INP NM=2,TEND=10.,NG=10,IALPH=1,R0=4.0,NDF=2,
      LABEL=17H BUILD UP 9404/AL $
P$SU IEOS=2,MAT=22,R2=1.,NCI=100,ME=1 $
P$ESC IBRN=3,BUD=.4,XV=3. $
P$BURN VCJ=.88,E=.187234 $
P$SU MAT=2,R2=0.,NCI=50,ME=1 $
P$ESC Y0=.00367,XMU=.256,XV=3.5 $
```



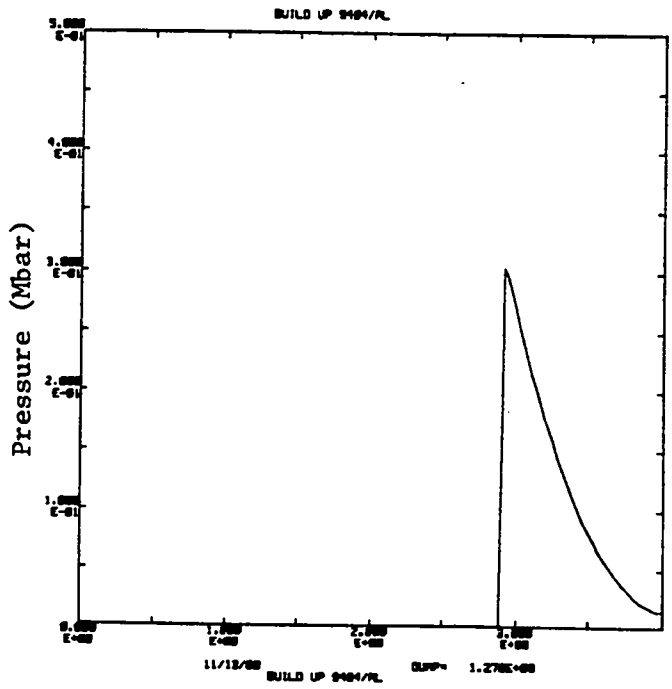
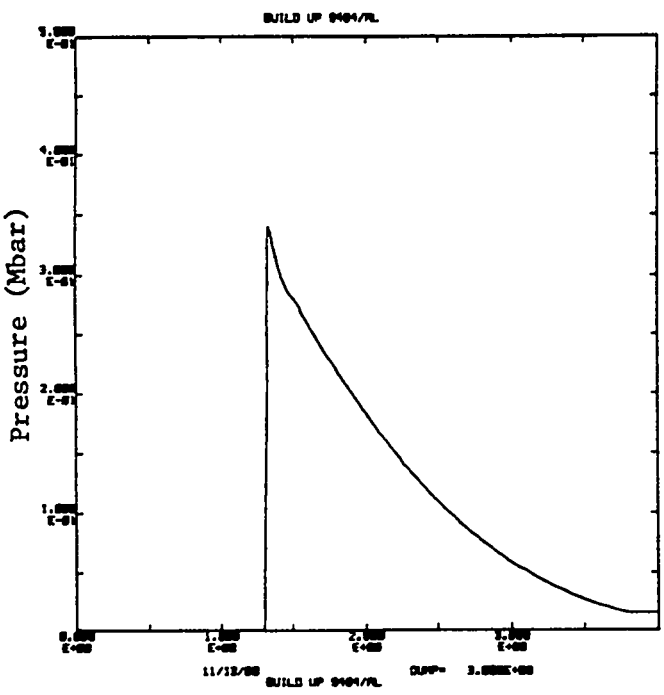
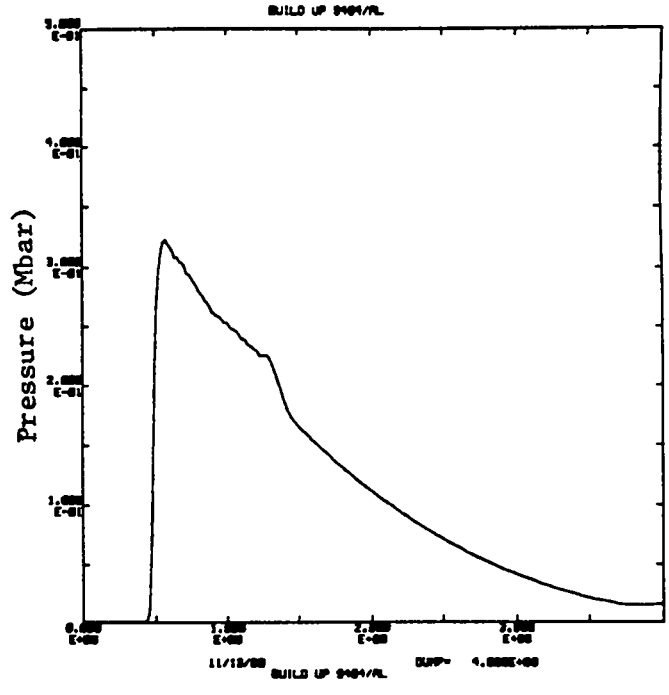


Fig. 11.
Pressure contours (0.020 Mbar) and Spall Layers.


Pressure (Mbar)
Distance (cm)


Pressure (Mbar)
Distance (cm)

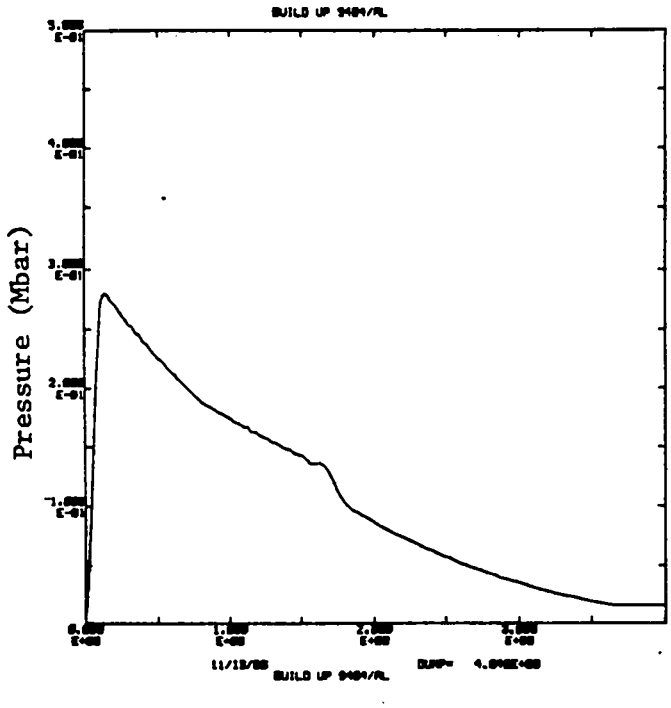

Pressure (Mbar)
Distance (cm)

Fig. 11. (cont)

D. 5 cm of Comp. B in the C-J Volume Burn Model Pushing 1 cm of Al with a SESAME Equation of State

Input File DATA

```
P$INP NM=2,RO=6.,IALPH=1,NG=20,TEND=8.,UI=-.213564,UF=.15,
      NMAX=10,NADD=2,
      LABEL=26H CJ BURN COMP B/SESAME AL $
P$SU MAT=19,R2=1.,NCI=100,ME=1 $
P$ESC IBRN=2,XV=2.5 $
P$BURN VCJ=.428513 $
P$SU IEOS=4,MAT=3710,NCI=25,R2=0.,ME=1 $
P$ESC XV=3. $
```

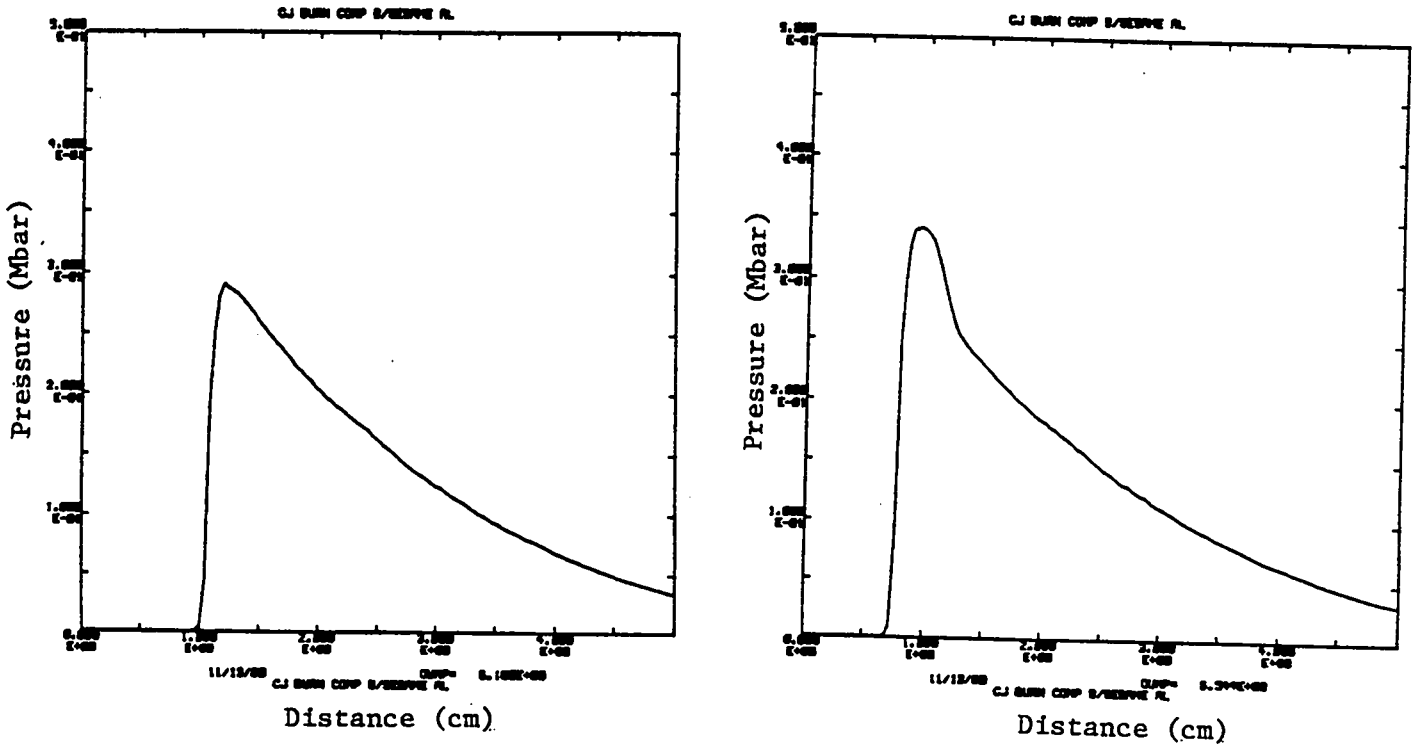


Fig. 12.

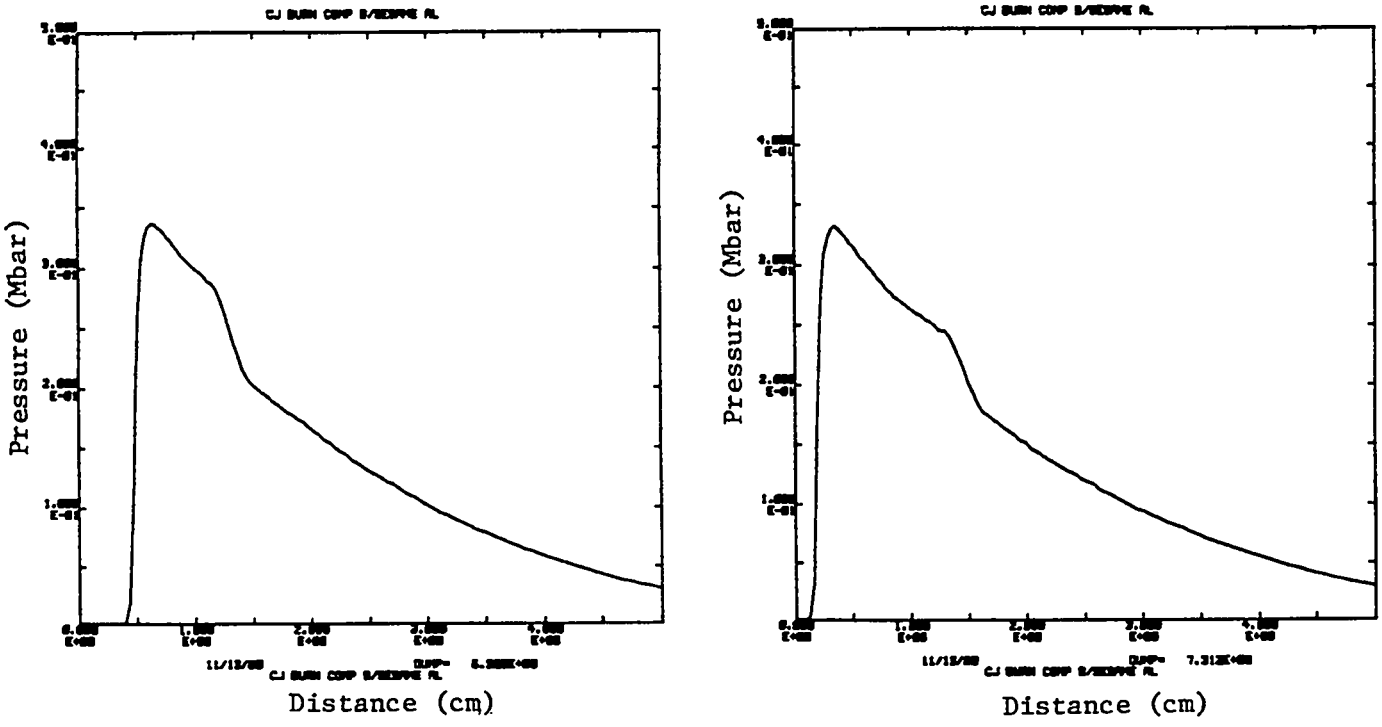


Fig. 12. (cont)

VI. HMLB AND SESAME EQUATION-OF-STATE LIBRARIES

In this section we discuss the use of the library HMLB for the HOM EOS and the SESAME tabular EOS library. Since the use of the HOM EOS can require the specification of many constants, we have provided a library of typical materials for metals, gases, and reacting materials. Any particular EOS constant in HMLB may be changed in HYDROX on the ESC NAMELIST since the library values are read first, and then the values specified in ESC are changed. Unspecified variables in ESC are thus defaulted to the values in HMLB. In Sec. A we give a list of the materials on HMLB, a cross-reference table of HYDROX and SIN variable names, and a listing of all the HMLB constants. Further information on the HOM EOS may be found in Ref. 2 of Sec. I.

HYDROX includes the capability of accessing the SESAME tabular EOS library and uses special subroutines for reading the library and doing the required numerical interpolation. In Sec. B we have merely listed the materials that are currently available. Reference 4 of Sec. I contains additional information about the SESAME library.

A. HMLB

HMLB is a library of constants for 29 different materials for use by the HOM equation of state in HYDROX. At LASL, HMLB may be obtained by the LTSS command:

```
MASS GET /HYDROX/HMLB
```

Before running HYDROX, HMLB must be obtained as a local file if the HOM EOS is used; IEOS=1 and MAT≠0 in the SU NAMELIST causes a search of HMLB for the material number specified by MAT.

1. Materials in the HMLB HOM EOS Library

```
 1  BE
 2  2024 AL
 3  NI
 4  COPPER
 5 STEEL
 6  TA
 7  AU
 8  LEAD
 9  U
10 301 POLYIMIDE
11  PLEXG
12  CH2
13  FOAM
14 AIR 1
15 AIR 2
16  BAHE
17 NQ ARRHENIUS
18 NQ FOREST FIRE
19  COMP B SHARP SHOCK
20  COMP B CJ(ARRH)
21 9404 CJ
22 9404 BUILD UP EOS
23 9404 GAMMA LAW
24 9404 FOREST FIRE
25 TATB/WAX FF F(P)
26 X0290 FF PCJ=.285
27 NQ/ESTANE 95/5 FF(T)
30 NQ FF RH ZERO ORDER
31  TNT
```

2. Cross-Reference Table Between HYDROX Variables and SIN Variables for HMLB

HYDROX	SIN
MAT	NMAT
---	IEXP
IBRN	IBRN
NV	IVIS
XV	VFACT
ROW	RHOØ
PØ	PØ
TØ	TØ
ZI	EØ
UØ	UØ
CI	SOL(1)

HYDROX	SIN
S1	SOL(2)
SWV	SOL(3)
C2	SOL(4)
S2	SOL(5)
FS	SOL(6)
GS	SOL(7)
HS	SOL(8)
SI	SOL(9)
SJ	SOL(10)
GAMMA	SOL(11)
CV	SOL(12)
VØ	SOL(13)
ALP	SOL(14)
SP	SOL(15)
USP	SOL(16)
TØ	SOL(17)
PØ	SOL(18)
YØ	SOL(19)
XMU	SOL(20)
PLAP	SOL(21)
---	SOL(22)
VMN	SOL(23)
WØ	WØ
Z	Z
E	E
VCJ	VCJ

HYDROX	SIN	
---	DCJ	
---	BCJUP	
ND	NDWDT	
PCJ	BPCJ	
PM	AMINP	
DWDT	DWDT	
GC	GAS	
A	GAS(1)	When the Barnes EOS is used
BR	GAS(2)	
BA	GAS(3)	
VBØ	GAS(4)	
VBSW	GAS(5)	
BUA	BUA	
BUB	BUB	
BUMAX	BUMAX	
BUDV	BUDV	

3. Listing of the EOS Constants in HMLB

```
$N
 NMAT   =        1,
 NN     =       -1,
$END
          *****  BE                    *****

$DAT
 IEXP   =        0,
 ISRN   =        0,
 IVIS   =        0,
 VFACT  =   2.0000000000000E+00,
 RHO0   =   1.8450000000000E+00,
 P0     =   1.0000000000000E-06,
 T0     =   3.0000000000000E+02,
 E0     =   0.                  ,
 U0     =   0.                  ,
 SOL    =   7.9750000000000E-01,    1.0910000000000E+00,
            1.0000000000000E-02,    0.                  ,
            0.                  ,    1.4949229523200E+01,
            3.4868986350100E+01,    3.9874001980200E+01,
            9.4841753554900E+00,   -1.9607277845000E+00,
            1.1800000000000E+00,    4.7400000000000E-01,
            5.4200542005400E-01,    1.2330000000000E-05,
            0.                  ,    0.                  ,
            3.0000000000000E+02,    1.0000000000000E-06,
            0.                  ,    0.                  ,
            0.                  ,    1.0000000000000E-06,
            0.                  ,
 W0     =   1.0000000000000E+00,
 Y      =   0.                  ,
 E      =   0.                  ,
 VCJ    =   0.                  ,
 DCJ    =   0.                  ,
 BCJUP  =   0.                  ,
 NDWDT  =        0,
 BPCJ   =   0.                  ,
 AMINP  =   0.                  ,
 DWDT   =   0.                  ,    0.                  ,
            0.                  ,    0.                  ,
            0.                  ,    0.                  ,
            0.                  ,    0.                  ,
            0.                  ,    0.                  ,
            0.                  ,    0.                  ,
            0.                  ,    0.                  ,
            0.                  ,    0.                  ,
            0.                  ,    0.                  ,
 GAS    =   0.                  ,    0.                  ,
            0.                  ,    0.                  ,
            0.                  ,    0.                  ,
            0.                  ,    0.                  ,
            0.                  ,    0.                  ,
            0.                  ,    0.                  ,
            0.                  ,    0.                  ,
            0.                  ,    0.                  ,
            0.                  ,
 BUA    =   0.                  ,
 BUB    =   0.                  ,
 BUMAX  =   0.                  ,
 BUDV   =   0.                  ,
$END
```

```
$N
 NMAT    =         2,
 NN      =        -1,
$END
          *****  2024 AL              *****


$DAT
 IEXP    =         0,
 IBRN    =         0,
 IVIS    =         0,
 VFACT   =    2.0000000000000E+00,
 RHOO    =    2.7850000000000E+00,
 PO      =    1.0000000000000E-06,
 TO      =    3.0000000000000E+02,
 EO      =    0.                  ,
 UO      =    0.                  ,
 SOL     =    5.3500000000000E-01,    1.3500000000000E+00,
              1.0000000000000E-01,    0.                  ,
              0.                  ,   -7.9611586687400E+01,
             -3.1753356163300E+02,   -4.3852537153300E+02,
             -2.6424824896000E+02,   -5.7973496473200E+01,
              1.7000000000000E+00,    2.2000000000000E-01,
              3.5906642728900E-01,    2.4000000000000E-05,
              7.1400000000000E-02,    5.0000000000000E-02,
              3.0000000000000E+02,    1.0000000000000E-06,
              0.                  ,   0.                  ,
              5.0000000000000E-02,    1.0000000000000E-06,
              0.                  ,
 WO      =    1.0000000000000E+00,
 Z       =    4.6000000000000E+03,
 E       =    9.5000000000000E+02,
 VCJ     =    0.                  ,
 DCJ     =    0.                  ,
 BCJUP   =    0.                  ,
 NDWDT   =         0,
 RPCJ    =    0.                  ,
 AMINP   =    0.                  ,
 DWDT    =    0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
 GAS     =    0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,
 BUA     =    0.                  ,
 BUB     =    0.                  ,
 BUMAX   =    0.                  ,
 BUDV    =    0.                  ,
$END
```

```
$N
 NMAT   =         3,
 NN     =        -1,
$END
        *****  NI                    *****


$DAT
 IEXP   =         0,
 IBRN   =         0,
 IVIS   =         0,
 VFACT  =    2.0000000000000E+00,
 RHOO   =    8.8600001000000E+00,
 PO     =    1.0000000000000E-06,
 TO     =    3.0000000000000E+02,
 EO     =    0.                  ,
 UO     =    0.                  ,
 SOL    =    4.6460000000000E-01,    1.4450000000000E+00,
             1.0000000000000E-02,    0.                  ,
             0.                  ,   -2.0354981593800E+03,
            -3.7098532585100E+03,   -2.5122620102000E+03,
            -7.5077048497800E+02,   -8.3468184762400E+01,
             1.8900000000000E+00,    1.0500000000000E-01,
             1.1286681715600E-01,    1.3000000000000E-05,
             0.                  ,   0.                  ,
             3.0000000000000E+02,    1.0000000000000E-06,
             0.                  ,   0.                  ,
             0.                  ,   1.0000000000000E-06,
             0.                  ,
 WO     =    1.0000000000000E+00,
 Z      =    0.                  ,
 E      =    0.                  ,
 VCJ    =    0.                  ,
 DCJ    =    0.                  ,
 BCJUP  =    0.                  ,
 NDWDT  =         0,
 BPCJ   =    0.                  ,
 AMINP  =    0.                  ,
 DWDT   =    0.                  ,   0.                  ,
             0.                  ,   0.                  ,
             0.                  ,   0.                  ,
             0.                  ,   0.                  ,
             0.                  ,   0.                  ,
             0.                  ,   0.                  ,
             0.                  ,   0.                  ,
             0.                  ,   0.                  ,
             0.                  ,   0.                  ,
             0.                  ,   0.                  ,
 GAS    =    0.                  ,   0.                  ,
             0.                  ,   0.                  ,
             0.                  ,   0.                  ,
             0.                  ,   0.                  ,
             0.                  ,   0.                  ,
             0.                  ,   0.                  ,
             0.                  ,   0.                  ,
             0.                  ,   0.                  ,
             0.                  ,   0.                  ,
             0.                  ,
 BUA    =    0.                  ,
 BUB    =    0.                  ,
 BUMAX  =    0.                  ,
 BUDV   =    0.                  ,
$END
```

```
$N
 NMAT    =         4,
 NN      =        -1,
$END
          *****  COPPER                *****


$DAT
 IEXP    =         0,
 IBRN    =         0,
 IVIS    =         0,
 VFACT   =    2.0000000000000E+00,
 RHOO    =    8.9030000000000E+00,
 PO      =    1.0000000000000E-06,
 TO      =    3.0000000000000E+02,
 EO      =    0.                  ,
 UO      =    0.                  ,
 SOL     =    3.9580000000000E-01,    1.4970000000000E+00,
              1.0000000000000E-03,    0.                  ,
              0.                  ,   -7.2269373246900E+02,
             -1.4234042687800E+03,   -1.0197498949400E+03,
             -3.1807912677400E+02,   -3.6471449881900E+01,
              2.0000000000000E+00,    9.3000000000000E-02,
              1.1232168931800E-01,    1.7670000000000E-05,
              1.0000000000000E-01,    1.2000000000000E-01,
              3.0000000000000E+02,    1.0000000000000E-06,
              3.0000000000000E-03,    4.6500000000000E-01,
              5.0000000000000E-02,    1.0000000000000E-06,
              0.                  ,
 WO      =    1.0000000000000E+00,
 Z       =    5.5700000000000E+03,
 F       =    1.3530000000000E+03,
 VCJ     =    0.                  ,
 DCJ     =    0.                  ,
 BCJUP   =    0.                  ,
 NDWDT   =         0,
 BPCJ    =    0.                  ,
 AMINP   =    0.                  ,
 DWDT    =    0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
 GAS     =    0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,
 BUA     =    0.                  ,
 BUB     =    0.                  ,
 BUMAX   =    0.                  ,
 BUDV    =    0.                  ,
$END
```

```
$N
 NMAT    =         5,
 NN      =        -1,
$END
          ***** STEEL                 *****


$DAT
 IEXP    =         0,
 IBRN    =         0,
 IVIS    =         0,
 VFACT   =    2.00000000000000E+00,
 RHOO    =    7.91700000000000E+00,
 PO      =    1.00000000000000E-06,
 TO      =    3.00000000000000E+02,
 EO      =    0.                   ,
 UO      =    0.                   ,
 SOL     =    4.58000000000000E-01,    1.51000000000000E+00,
              1.00000000000000E-02,    0.                   ,
              0.                   ,   -3.82382587453000E+03,
             -7.03211954024000E+03,   -4.82670213894000E+03,
             -1.46678402118000E+03,   -1.66391615983000E+02,
              2.00000000000000E+00,    1.07000000000000E-01,
              1.26310471138000E-01,    1.17000000000000E-05,
              0.                   ,    0.                   ,
              3.00000000000000E-02,    1.00000000000000E-06,
              0.                   ,    0.                   ,
              0.                   ,    1.00000000000000E-06,
              0.                   ,
 WO      =    1.00000000000000E+00,
 Z       =    0.                   ,
 E       =    0.                   ,
 VCJ     =    0.                   ,
 DCJ     =    0.                   ,
 BCJUP   =    0.                   ,
 NDWDT   =         0,
 BPCJ    =    0.                   ,
 AMINP   =    0.                   ,
 DWDT    =    0.                   ,    0.                   ,
              0.                   ,    0.                   ,
              0.                   ,    0.                   ,
              0.                   ,    0.                   ,
              0.                   ,    0.                   ,
              0.                   ,    0.                   ,
              0.                   ,    0.                   ,
              0.                   ,    0.                   ,
              0.                   ,    0.                   ,
              0.                   ,    0.                   ,
 GAS     =    0.                   ,    0.                   ,
              0.                   ,    0.                   ,
              0.                   ,    0.                   ,
              0.                   ,    0.                   ,
              0.                   ,    0.                   ,
              0.                   ,    0.                   ,
              0.                   ,    0.                   ,
              0.                   ,    0.                   ,
              0.                   ,
 BUA     =    0.                   ,
 BUB     =    0.                   ,
 BUMAX   =    0.                   ,
 BUDV    =    0.                   ,
$END
```

```
$N
 NMAT   =         6,
 NN     =        -1,
$END
          *****  TA                    *****


$DAT
 IEXP   =         0,
 IRRN   =         0,
 IVIS   =         0,
 VFACT  =    2.0000000000000E+00,
 RHOO   =    1.6690000000000E+01,
 PO     =    1.0000000000000E-06,
 TO     =    3.0000000000000E+02,
 EO     =    0.                    ,
 UO     =    0.                    ,
 SOL    =    3.4140000000000E-01,    1.2010000000000E+00,
             1.0000000000000E-02,    0.                  ,
             0.                  ,   -2.7769235055300E+03,
            -4.0152531315500E+03,   -2.1587503349800E+03,
            -5.1221616258700E+02,   -4.5223258682200E+01,
             1.7000000000000E+00,    3.3000000000000E-02,
             5.9916117435600E-02,    1.6590000000000E-05,
             0.                  ,   0.                  ,
             3.0000000000000E+02,    1.0000000000000E-06,
             4.0000000000000E-03,    7.0500000000000E-01,
             5.0000000000000E-02,    0.                  ,
             0.                  ,
 WO     =    1.0000000000000E+00,
 Z      =    5.0000000000000E+03,
 E      =    3.2700000000000E+03,
 VOJ    =    0.                    ,
 DOJ    =    0.                    ,
 ROJUP  =    0.                    ,
 NDWDT  =         0,
 BPOJ   =    0.                    ,
 AMINP  =    0.                    ,
 DWDT   =    0.                    ,   0.                  ,
             0.                    ,   0.                  ,
             0.                    ,   0.                  ,
             0.                    ,   0.                  ,
             0.                    ,   0.                  ,
             0.                    ,   0.                  ,
             0.                    ,   0.                  ,
             0.                    ,   0.                  ,
             0.                    ,   0.                  ,
             0.                    ,   0.                  ,
 GAS    =    0.                    ,   0.                  ,
             0.                    ,   0.                  ,
             0.                    ,   0.                  ,
             0.                    ,   0.                  ,
             0.                    ,   0.                  ,
             0.                    ,   0.                  ,
             0.                    ,   0.                  ,
             0.                    ,   0.                  ,
             0.                    ,
 BUA    =    0.                    ,
 BUB    =    0.                    ,
 BUMAX  =    0.                    ,
 BUDV   =    0.                    ,
$END
```

```
$N
 NMAT    =         7,
 NN      =        -1,
$END
          *****  AU                    *****


$DAT
 IEXP    =         0,
 IBRN    =         0,
 IVIS    =         0,
 VFACT   =    2.0000000000000E+00,
 RHOO    =    1.9240000000000E+01,
 PO      =    1.0000000000000E-06,
 TO      =    3.0000000000000E+02,
 EO      =    0.                    ,
 UO      =    0.                    ,
 SOL     =    3.0750000000000E-01,    1.5600000000000E+00,
              1.0000000000000E-02,    0.                  ,
              0.                  ,   -3.8649405250300E+03,
             -5.1941782941600E+03,   -2.6112896415500E+03,
             -5.8203419236900E+02,   -4.8455143294100E+01,
              2.0000000000000E+00,    3.1200000000000E-02,
              5.1975051970000E-02,    1.4200000000000E-05,
              0.                  ,   0.                  ,
              3.0000000000000E+02,    1.0000000000000E-06,
              0.                  ,   0.                  ,
              5.0000000000000E-02,    0.                  ,
              0.                  ,
 WO      =    1.0000000000000E+00,
 Z       =    5.0000000000000E+03,
 E       =    1.3360000000000E+03,
 VCJ     =    0.                    ,
 DCJ     =    0.                    ,
 RCJUP   =    0.                    ,
 NDWDT   =         0,
 BPCJ    =    0.                    ,
 AMINP   =    0.                    ,
 DWDT    =    0.                    ,   0.                  ,
              0.                    ,   0.                  ,
              0.                    ,   0.                  ,
              0.                    ,   0.                  ,
              0.                    ,   0.                  ,
              0.                    ,   0.                  ,
              0.                    ,   0.                  ,
              0.                    ,   0.                  ,
              0.                    ,   0.                  ,
              0.                    ,   0.                  ,
 GAS     =    0.                    ,   0.                  ,
              0.                    ,   0.                  ,
              0.                    ,   0.                  ,
              0.                    ,   0.                  ,
              0.                    ,   0.                  ,
              0.                    ,   0.                  ,
              0.                    ,   0.                  ,
              0.                    ,   0.                  ,
              0.                    ,
 BUA     =    0.                    ,
 BUB     =    0.                    ,
 BUMAX   =    0.                    ,
 BUDV    =    0.                    ,
$END
```

```
$N
 NMAT    =         8,
 NN      =        -1,
$END
         *****  LEAD                 *****


$DAT
 IEXP    =         0,
 IBRN    =         0,
 IVIS    =         0,
 VFACT   =    2.0000000000000E+00,
 RHOO    =    1.1340000000000E+01,
 PO      =    1.0000000000000E-06,
 TO      =    3.0000000000000E+02,
 EO      =    0.                  ,
 UO      =    0.                  ,
 SOL     =    2.0280000000000E-01,    1.5170000000000E+00,
              1.0000000000000E-03,    0.                  ,
              0.                  ,    3.9729257221900E+02,
              4.4550742326900E+02,    1.6992751638400E+02,
              2.2953413952900E+01,    4.9665122596100E-01,
              2.0340000000000E+00,    3.0000000000000E-02,
              8.9183421516800E-02,    2.8370000000000E-05,
              1.0000000000000E-01,    2.0000000000000E-02,
              3.0000000000000E+02,    1.0000000000000E-06,
              0.                  ,    0.                  ,
              0.                  ,    1.0000000000000E-06,
              0.                  ,
 WO      =    1.0000000000000E+00,
 Y       =    3.5000000000000E+03,
 E       =    5.9900000000000E+02,
 VCJ     =    0.                  ,
 DCJ     =    0.                  ,
 RCJUP   =    0.                  ,
 NDWDT   =         0,
 BPCJ    =    0.                  ,
 AMINP   =    0.                  ,
 DWDT    =    0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
 GAS     =    0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,
 BUA     =    0.                  ,
 BUB     =    0.                  ,
 BUMAX   =    0.                  ,
 BUDV    =    0.                  ,
$END
```

```
$N
 NMAT    =         9,
 NN      =        -1,
$END
          *****  U                    *****


$DAT
 IEXP    =         0,
 IBRN    =         0,
 IVIS    =         0,
 VFACT   =    2.0000000000000E+00,
 RHO0    =    1.8910000000000E+01,
 P0      =    1.0000000000000E-06,
 T0      =    3.0000000000000E+02,
 E0      =    0.                  ,
 U0      =    0.                  ,
 SIL     =    2.5400000000000E-01,    1.5000000000000E+00,
              1.0000000000000E-04,    0.                  ,
              0.                  ,    8.1777341466300E+02,
              6.1009951139000E+02,    9.0904269245400E+01,
             -2.2037316277600E+01,   -4.8735636843100E+00,
              2.0000000000000E+00,    2.7600000000000E-02,
              5.2882072000000E-02,    1.1660000000000E-05,
              0.                  ,    0.                  ,
              3.0000000000000E+02,    1.0000000000000E-06,
              0.                  ,    0.                  ,
              0.                  ,    1.0000000000000E-06,
              0.                  ,
 WO      =    1.0000000000000E+00,
 Z       =    0.                  ,
 E       =    0.                  ,
 VCJ     =    0.                  ,
 DCJ     =    0.                  ,
 BCJUP   =    0.                  ,
 NDWDT   =         0,
 BPCJ    =    0.                  ,
 AMINP   =    0.                  ,
 DWDT    =    0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
 GAS     =    0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,
 BUA     =    0.                  ,
 BUB     =    0.                  ,
 BUMAX   =    0.                  ,
 BUDV    =    0.                  ,
$END
```

```
$N
 NMAT    =        10,
 NN      =        -1,
$END
        ***** 301 POLYIMIDE        *****

$DAT
 IEXP    =         0,
 IBRN    =         0,
 IVIS    =         2,
 VFACT   =    2.0000000000000E-03,
 RHOO    =    1.4140000000000E+00,
 PO      =    0.                  ,
 TO      =    3.0000000000000E+02,
 EO      =    0.                  ,
 UO      =    0.                  ,
 SOL     =    2.6500000000000E-01,    1.5100000000000E+00,
              4.4878000000000E-01,    4.9000000000000E-01,
              4.6860000000000E-01,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              1.0000000000000E+00,    2.5000000000000E-01,
              7.0721357850000E-01,    1.0000000000000E-05,
              0.                  ,    0.                  ,
              3.0000000000000E+02,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              4.4878000000000E-01,
 WO      =    1.0000000000000E+00,
 Z       =    0.                  ,
 E       =    0.                  ,
 VCJ     =    0.                  ,
 DCJ     =    0.                  ,
 BCJUP   =    0.                  ,
 NDWDT   =         0,
 BPCJ    =    0.                  ,
 AMINP   =    0.                  ,
 DWDT    =    0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
 GAS     =    0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,
 BUA     =    0.                  ,
 BUB     =    0.                  ,
 BUMAX   =    0.                  ,
 BUDV    =    0.                  ,
$END
```

```
$N
 NMAT    =        11,
 NN      =        -1,
$END
          *****  PLEXG                *****


$DAT
 IEXP    =         0,
 IBRN    =         0,
 IVIS    =         0,
 VFACT   =    2.0000000000000E+00,
 RHOO    =    1.1800000000000E+00,
 PO      =    1.0000000000000E-06,
 TO      =    3.0000000000000E+02,
 EO      =    0.                    ,
 UO      =    0.                    ,
 SOL     =    2.4320000000000E-01,    1.5785000000000E+00,
              1.0000000000000E-04,    0.                  ,
              0.                  ,    5.2938024350600E+00,
             -4.2495037136800E+00,   -1.5505557633200E+01,
             -3.0863807557200E+01,   -1.4670819373900E+01,
              1.0000000000000E+00,    3.5000000000000E-01,
              8.4745762700000E-01,    1.0000000000000E-04,
              1.0000000000000E+02,    1.0000000000000E+00,
              3.0000000000000E+02,    1.0000000000000E-06,
              0.                  ,    0.                  ,
              0.                  ,    1.0000000000000E-06,
              0.                  ,
 WO      =    1.0000000000000E+00,
 Z       =    0.                    ,
 E       =    0.                    ,
 VCJ     =    0.                    ,
 DCJ     =    0.                    ,
 BCJUP   =    0.                    ,
 NDWDT   =         0,
 BPCJ    =    0.                    ,
 AMINP   =    0.                    ,
 DWDT    =    0.                    ,    0.                  ,
              0.                    ,    0.                  ,
              0.                    ,    0.                  ,
              0.                    ,    0.                  ,
              0.                    ,    0.                  ,
              0.                    ,    0.                  ,
              0.                    ,    0.                  ,
              0.                    ,    0.                  ,
              0.                    ,    0.                  ,
              0.                    ,    0.                  ,
 GAS     =    0.                    ,    0.                  ,
              0.                    ,    0.                  ,
              0.                    ,    0.                  ,
              0.                    ,    0.                  ,
              0.                    ,    0.                  ,
              0.                    ,    0.                  ,
              0.                    ,    0.                  ,
              0.                    ,    0.                  ,
              0.                    ,
 BUA     =    0.                    ,
 BUB     =    0.                    ,
 BUMAX   =    0.                    ,
 BUDV    =    0.                    ,
$END
```

```
$N
 NMAT    =        12,
 NN      =        -1,
$END
          *****  CH2                    *****


$DAT
 IEXP    =         0,
 IBRN    =         0,
 IVIS    =         0,
 VFACT   =    2.0000000000000E+00,
 RHOO    =    9.1500000000000E-01,
 PO      =    1.0000000000000E-06,
 TO      =    3.0000000000000E+02,
 EO      =    0.                    ,
 UO      =    0.                    ,
 SOL     =    2.9010000000000E-01,    1.4810000000000E+00,
              1.0000000000000E-02,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              5.0000000000000E-01,    5.0000000000000E-01,
              1.0928961750000E+00,    1.0000000000000E-04,
              0.                    ,    0.                    ,
              3.0000000000000E+02,    1.0000000000000E-06,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,
 WO      =    1.0000000000000E+00,
 Z       =    0.                    ,
 E       =    0.                    ,
 VCJ     =    0.                    ,
 DCJ     =    0.                    ,
 PCJUP   =    0.                    ,
 NDWDT   =         0,
 RPCJ    =    0.                    ,
 AMINP   =    0.                    ,
 DWDT    =    0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
 GAS     =    0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,
 BUA     =    0.                    ,
 BUB     =    0.                    ,
 BUMAX   =    0.                    ,
 BUDV    =    0.                    ,
$END
```

```
$N
 NMAT   =        13,
 NN     =        -1,
$END
         *****  FOAM                  *****


$DAT
 IEXP   =         1,
 IBRN   =         1,
 IVIS   =         0,
 VFACT  =    2.0000000000000E+00,
 RHOO   =    2.5600000000000E-01,
 PO     =    1.0000000000000E-06,
 TO     =    3.0000000000000E+02,
 EO     =    0.                  ,
 UO     =    0.                  ,
 SOL    =    1.0000000000000E-02,    1.4000000000000E+00,
             1.0000000000000E-03,    0.                  ,
             0.                  ,    5.7795005289400E+00,
             6.5738798524400E-01,    5.2908852170300E+00,
            -3.2818147067500E+01,    3.7389900213800E+01,
             1.0000000000000E-01,    5.0000000000000E-01,
             3.9062500000000E+00,    1.0000000000000E-05,
             0.                  ,    0.                  ,
             3.0000000000000E+02,    1.0000000000000E-06,
             0.                  ,    0.                  ,
             0.                  ,    0.                  ,
             0.                  ,
 WO     =    1.0000000000000E+00,
 Z      =    0.                  ,
 E      =    0.                  ,
 VCJ    =    2.5000000000000E+00,
 DCJ    =    2.5000000000000E+00,
 RCJUP  =    0.                  ,
 NDWDT  =         0,
 BPCJ   =    0.                  ,
 AMINP  =    0.                  ,
 DWDT   =    0.                  ,    0.                  ,
             0.                  ,    0.                  ,
             0.                  ,    0.                  ,
             0.                  ,    0.                  ,
             0.                  ,    0.                  ,
             0.                  ,    0.                  ,
             0.                  ,    0.                  ,
             0.                  ,    0.                  ,
             0.                  ,    0.                  ,
             0.                  ,    0.                  ,
 GAS    =   -2.3056290298900E+00,   -2.0327298176000E+00,
             4.1624706382900E-02,   -8.5046298250600E-03,
             1.3710841934300E-02,   -8.1341769155800E-01,
             3.5139377096100E-01,    3.4051522790100E-02,
             8.4954254906300E-04,   -2.6165006722900E-05,
             8.5358524401000E+00,   -4.8068713991300E-01,
            -1.0822141051100E-01,    6.4680172755100E-02,
             9.1399439066400E-03,    5.0000000000000E-01,
             1.0000000000000E-01,
 BUA    =    0.                  ,
 BUB    =    0.                  ,
 BUMAX  =    0.                  ,
 BUDV   =    0.                  ,
$END
```

```
$N
 NMAT    =        14,
 NN      =        -1,
$END
          ***** AIR 1                    *****


$DAT
 IEXP    =         1,
 IBRN    =         0,
 IVIS    =         0,
 VFACT   =    1.0000000000000E-02,
 R400    =    2.2022200000000E-03,
 PO      =    1.1000000000000E-05,
 TO      =    3.0000000000000E+02,
 EO      =    3.0000000000000E-03,
 UO      =    0.                    ,
 SOL     =    0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              4.5408723000000E+02,       1.0000000000000E-05,
              0.                    ,    0.                    ,
              3.0000000000000E+02,       1.1000000000000E-05,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,
 WO      =    0.                    ,
 Z       =    0.                    ,
 E       =    0.                    ,
 VCJ     =    0.                    ,
 DCJ     =    0.                    ,
 BCJUP   =    0.                    ,
 NDWDT   =         0,
 BPCJ    =    0.                    ,
 AMINP   =    0.                    ,
 DWDT    =    0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
 GAS     =   -6.4815597907600E-01,      -2.3284494242200E+00,
              2.2211209300100E-01,      -8.8771800708400E-03,
             -1.7838446631100E-03,      -1.7128377158500E-01,
              3.5923780267100E-01,       2.4989330519100E-02,
              1.6963777637300E-03,       7.3978993872900E-05,
              8.7130933986300E+00,      -4.8115967696200E-01,
              4.7902390066100E-02,       5.9890749038100E-03,
             -2.1837533877900E-03,       5.0000000000000E-01,
              1.0000000000000E-01,
 BUA     =    0.                    ,
 BUB     =    0.                    ,
 BUMAX   =    0.                    ,
 BUDV    =    0.                    ,
$END
```

```
$N
 NMAT    =        15,
 NN      =        -1,
$END
          ***** AIR 2                ******


$DAT
 IEXP    =         1,
 IBRN    =         0,
 IVIS    =         1,
 VFACT   =    2.0000000000000E-01,
 RHOO    =    9.2462900000000E-04,
 PO      =    6.0000000000000E-07,
 TO      =    3.0000000000000E+02,
 EO      =    2.4668800000000E-03,
 UO      =    0.                    ,
 SOL     =    0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              9.2965314640000E+02,    0.                    ,
              0.                    ,    0.                    ,
              3.0000000000000E+02,    1.0000000000000E-06,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,
 WO      =    0.                    ,
 Z       =    0.                    ,
 E       =    0.                    ,
 VCJ     =    0.                    ,
 DCJ     =    0.                    ,
 BCJUP   =    0.                    ,
 NDWDT   =         0,
 BPCJ    =    0.                    ,
 AMINP   =    0.                    ,
 DWDT    =    0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
 GAS     =   -4.5925651463400E+00,   -9.1684449125200E-01,
             -2.1288704554600E-01,    5.4146702954700E-02,
             -4.6651572500600E-03,   -1.6181507888800E+00,
              8.5966902857500E-02,    1.6688939090600E-03,
             -1.2702592247200E-04,   -3.4388375401000E-06,
              8.1411219425200E+00,    1.0099419080700E-01,
             -2.1837686705400E-01,    5.4901424967700E-02,
             -4.7035249074400E-03,    5.0000000000000E-01,
              1.0000000000000E-01,
 BUA     =    0.                    ,
 BUB     =    0.                    ,
 BUMAX   =    0.                    ,
 BUDV    =    0.                    ,
$END
```

```
$N
 NMAT    =        16,
 NN      =        -1,
$END
         *****  BARE                 *****


$DAT
 IEXP    =         1,
 IBRN    =         3,
 IVIS    =         1,
 VFACT   =    2.0000000000000E+00,
 RHO0    =    2.6040000000000E+00,
 P0      =    1.0000000000000E-06,
 T0      =    3.0000000000000E+02,
 E0      =    0.                  ,
 U0      =    0.                  ,
 SOL     =    2.7150000000000E-01,   2.5760000000000E+00,
              1.0000000000000E-01,   0.                  ,
              0.                  ,  -8.6661849555200E+00,
             -5.8313782208900E+01,   -6.9716341085000E+01,
             -8.2009910278300E+00,   2.0719556900800E+01,
              6.7470000000000E-01,   4.0000000000000E-01,
              3.8402457700000E-01,   5.0000000000000E-05,
              0.                  ,  0.                  ,
              3.0000000000000E+02,   1.0000000000000E-06,
              0.                  ,  0.                  ,
              0.                  ,  0.                  ,
              0.                  ,
 WO      =    1.0000000000000E+00,
 Z       =    0.                  ,
 E       =    0.                  ,
 VCJ     =    4.8800000000000E-01,
 DCJ     =    4.8800000000000E-01,
 BCJUP   =    0.                  ,
 NOWDT   =         0,
 BPCJ    =    0.                  ,
 AMINP   =    0.                  ,
 DWDT    =    0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
 GAS     =   -6.2035295000000E+00,  -3.4936691000000E+00,
              0.                  ,   0.                  ,
              0.                  ,  -2.1397597000000E+00,
              4.3255033000000E-01,   8.5046596000000E-02,
              7.6787070000000E-03,   2.6461528000000E-04,
              0.                  ,  -1.4300000000000E+00,
              0.                  ,   0.                  ,
              0.                  ,   5.0000000000000E-01,
              6.0000000000000E-02,
 BUA     =    0.                  ,
 BUB     =    0.                  ,
 BUMAX   =    0.                  ,
 BUDV    =    0.                  ,
$END
```

```
$N
 NMAT   =        17,
 NN     =        -1,
$END
          ***** NO ARRHENIUS          *****


$DAT
 IEXP   =         1,
 IGRN   =         0,
 IVIS   =         1,
 VFACT  =    4.0000000000000E-01,
 RHOO   =    1.7140010000000E+00,
 PO     =    1.0000000000000E-06,
 TO     =    3.0000000000000E+02,
 EO     =    0.                    ,
 UO     =    0.                    ,
 SOL    =    2.3440000000000E-01,    1.7500000000000E+00,
             1.0000000000000E-06,    0.                  ,
             0.                    ,-4.3375662728300E+00,
            -5.2901710589600E+01,   -1.0134141654400E+02,
            -8.1576457053800E+01,   -2.1688340014100E+01,
             5.0000000000000E-01,    1.0000000000000E+00,
             5.8343057000000E-01,    5.0000000000000E-05,
             0.                    ,0.                  ,
             3.0000000000000E+02,    1.0000000000000E-06,
             0.                    ,0.                  ,
             0.                    ,1.0000000000000E-06,
             0.                    ,
 WO     =    1.0000000000000E+00,
 Z      =    0.                    ,
 E      =    4.5000000000000E+04,
 VCJ    =    0.                    ,
 DCJ    =    0.                    ,
 BCJUP  =    0.                    ,
 NDWDT  =         0,
 BPCJ   =    0.                    ,
 AMINP  =    0.                    ,
 DWDT   =    0.                    ,   0.                  ,
             0.                    ,   0.                  ,
             0.                    ,   0.                  ,
             0.                    ,   0.                  ,
             0.                    ,   0.                  ,
             0.                    ,   0.                  ,
             0.                    ,   0.                  ,
             0.                    ,   0.                  ,
             0.                    ,   0.                  ,
             0.                    ,   0.                  ,
 GAS    =   -3.7984107052400E+00,   -3.0340338334900E+00,
             1.3602389047600E-01,   -1.4409992462100E-01,
            -1.6149804591500E-01,   -1.6059840383600E+00,
             5.1283010050500E-01,    7.7617166547600E-02,
             3.8767269529200E-03,   -5.9008825467300E-05,
             7.2000000000000E+00,   -8.8963147931300E-01,
            -1.7250193817700E-01,   -1.3076342573300E-01,
            -1.5260936054800E-01,    5.0000000000000E-01,
             1.0000000000000E-01,
 BUA    =    0.                    ,
 BUB    =    0.                    ,
 BUMAX  =    0.                    ,
 BUDV   =    0.                    ,
$END
```

```
$N
 NMAT    =        18,
 NN      =        -1,
$END
          ***** NQ FOREST FIRE       *****


$DAT
 IEXP    =         1,
 IBRN    =         4,
 IVIS    =         1,
 VFACT   =    4.00000000000000E-01,
 RHOO    =    1.69900000000000E+00,
 PO      =    1.00000000000000E-06,
 TO      =    3.00000000000000E+02,
 EO      =    0.                   ,
 UO      =    0.                   ,
 SOL     =    3.00000000000000E-01,    1.79500000000000E+00,
              0.                   ,    0.                   ,
              0.                   ,   -4.33756627283000E+00,
             -5.29817105895000E+01,   -1.01341416544000E+02,
             -8.15764570538000E+01,   -2.16883400141000E+01,
              1.50000000000000E+00,    1.00000000000000E+00,
              5.88581510000000E-01,    5.00000000000000E-05,
              0.                   ,    0.                   ,
              3.00000000000000E+02,    1.00000000000000E-06,
              0.                   ,    0.                   ,
              0.                   ,    0.                   ,
              0.                   ,
 WO      =    1.00000000000000E+00,
 Z       =    0.                   ,
 E       =    0.                   ,
 VCJ     =    0.                   ,
 DCJ     =    0.                   ,
 BCJUP   =    0.                   ,
 NDWDT   =        15,
 BPCJ    =    2.90000000000000E-01,
 AMINP   =    5.00000000000000E-02,
 DWDT    =    4.92023896225000E+13,   -1.12335453055000E+14,
              1.16976394736000E+14,   -7.35591802150000E+13,
              3.11733466629000E+13,   -9.40731573405000E+12,
              2.08222889284000E+12,   -3.42977442078000E+11,
              4.21899479997000E+10,   -3.85113391834000E+09,
              2.56295657125000E+08,   -1.20223340488000E+07,
              3.73046757058000E+05,   -6.61730535643000E+03,
              3.35111799370000E+01,    0.                   ,
              0.                   ,    0.                   ,
              0.                   ,    0.                   ,
 GAS     =   -3.78132232236000E+00,   -2.86690722895000E+00,
              4.57803766659000E-01,   -2.13934760048000E-01,
             -3.87596501398000E-01,   -1.58138142170000E+00,
              5.33538344114000E-01,    9.10386245891000E-02,
              7.32482741070000E-03,    2.34366498224000E-04,
              6.70274815054000E+00,   -6.66940757461000E-01,
              1.71721541496000E-01,   -2.36545708591000E-01,
             -3.83605745852000E-01,    5.00000000000000E-01,
              1.00000000000000E-01,
 BUA     =    0.                   ,
 BUB     =    0.                   ,
 BUMAX   =    0.                   ,
 BUDV    =    0.                   ,
$END
```

```
$N
 NMAT    =        19,
 NN      =        -1,
$END
          *****  COMP B SHARP SHOCK  *****


$DAT
 IEXP    =         1,
 IRRN    =         3,
 IVIS    =         0,
 VFACT   =    3.5000000000000E+00,
 RHOO    =    1.7130000000000E+00,
 PO      =    1.0000000000000E-06,
 TO      =    3.0000000000000E+02,
 EO      =    0.                  ,
 UO      =    0.                  ,
 SOL     =    2.4000000000000E-01,    2.5500000000000E+00,
              1.0000000000000E-03,    0.                  ,
              0.                  ,   -9.3035923780500E+00,
             -7.3193114947300E+01,   -1.1984909720700E+02,
             -6.5549768378000E+01,    8.8811032659100E-01,
              8.0000000000000E-01,    2.5900000000000E-01,
              5.8309037900000E-01,    5.0000000000000E-05,
              0.                  ,    0.                  ,
              3.0000000000000E+02,    1.0000000000000E-06,
              0.                  ,    0.                  ,
              0.                  ,    1.0000000000000E-06,
              0.                  ,
 WO      =    1.0000000000000E+00,
 Z       =    0.                  ,
 E       =    0.                  ,
 VCJ     =    6.0300000000000E-01,
 DCJ     =    8.0300000000000E-01,
 BCJUP   =    0.                  ,
 NDWDT   =         0,
 BPCJ    =    0.                  ,
 AMINP   =    0.                  ,
 DWDT    =    0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
 GAS     =   -3.5630947234000E+00,   -2.7600000000000E+00,
              0.                  ,    0.                  ,
              0.                  ,   -1.5607327324500E+00,
              5.1979454280200E-01,    6.7891598954500E-02,
              3.2585940953600E-03,    2.2708937422000E-05,
              0.                  ,   -5.5226424100000E-01,
              0.                  ,    0.                  ,
              0.                  ,    5.0000000000000E-01,
              1.0000000000000E-01,
 BUA     =    0.                  ,
 BUB     =    0.                  ,
 BUMAX   =    0.                  ,
 BUDV    =    0.                  ,
$END
```

```
$N
 NMAT    =        20,
 NN      =        -1,
$END
          *****  COMP B CJ(ARRH)     *****


$DAT
 IEXP    =         1,
 IBRN    =         1,
 IVIS    =         0,
 VFACT   =    3.5000000000000E+00,
 R400    =    1.7300000000000E+00,
 PO      =    1.0000000000000E-06,
 TO      =    3.0000000000000E+02,
 EO      =    0.                  ,
 UO      =    0.                  ,
 SOL     =    2.3100000000000E-01,    1.8300000000000E+00,
              1.0000000000000E-02,    0.                  ,
              0.                  ,   -8.6482257659700E+00,
             -7.6497948971400E+01,   -1.4880798590100E+02,
             -1.2260687862300E+02,   -3.4139045857900E+01,
              2.0000000000000E+00,    2.5000000000000E-01,
              5.7803468200000E-01,    5.0000000000000E-05,
              0.                  ,   0.                  ,
              3.0000000000000E+02,    1.0000000000000E-06,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,
 WO      =    1.0000000000000E+00,
 Z       =    1.0000000000000E+13,
 E       =    4.5000000000000E+04,
 VCJ     =    4.3311700000000E-01,
 DCJ     =    4.3311700000000E-01,
 RCJUP   =    0.                  ,
 NDWDT   =         0,
 SPCJ    =    0.                  ,
 AMINP   =    0.                  ,
 DWDT    =    0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
 GAS     =   -3.8101492210200E+00,   -2.9887450000000E+00,
              0.                  ,   0.                  ,
              0.                  ,   -1.5935241619500E+00,
              5.0113382815600E-01,    7.8549138663000E-02,
              5.3425796030900E-03,    1.2783948755700E-04,
              7.5081772908100E+00,   -4.5925899205700E-01,
              5.8670140664100E-02,    2.1435450837900E-02,
             -7.0630889677900E-03,    5.0000000000000E-01,
              1.0000000000000E-01,
 BUA     =    0.                  ,
 BUB     =    0.                  ,
 BUMAX   =    0.                  ,
 BUDV    =    0.                  ,
$END
```

```
$N
 NMAT    =        21,
 NN      =        -1,
$END
          ***** 9404 CJ                ******


$DAT
 IEXP    =         1,
 IBRN    =         1,
 IVIS    =         0,
 VFACT   =    1.5000000000000E+00,
 RHOO    =    1.8440000000000E+00,
 PO      =    1.0000000000000E-06,
 TO      =    3.0000000000000E+02,
 EO      =    0.                    ,
 UO      =    0.                    ,
 SOL     =    2.7150000000000E-01,    2.5760000000000E+00,
              1.0000000000000E-01,    0.                    ,
              0.                    ,  -8.6661849555200E+00,
             -5.8313732209900E+01,    -6.9716341085000E+01,
             -8.2009910278300E+00,     2.0719556900800E+01,
              6.7470000000000E-01,     4.0000000000000E-01,
              5.4229935000000E-01,     5.0000000000000E-05,
              0.                    ,  0.                    ,
              3.0000000000000E+02,     1.0000000000000E-06,
              0.                    ,  0.                    ,
              0.                    ,  1.0000000000000E-06,
              0.                    ,
 WO      =    1.0000000000000E+00,
 Y       =    0.                    ,
 E       =    0.                    ,
 VCJ     =    4.1318000000000E-01,
 DCJ     =    4.1318000000000E-01,
 BCJUP   =    0.                    ,
 NDWDT   =         0,
 BPCJ    =    0.                    ,
 AMINP   =    0.                    ,
 DWDT    =    0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
              0.                    ,    0.                    ,
 GAS     =   -3.9071763513500E+00,    -3.2000000000000E+00,
              0.                    ,    0.                    ,
              0.                    ,   -1.6380521783900E+00,
              5.2133755898000E-01,     8.5757555184200E-02,
              6.2392162210300E-03,     1.6563329597600E-04,
              0.                    ,  -1.1086600000000E+00,
              0.                    ,    0.                    ,
              0.                    ,    5.0000000000000E-01,
              1.0000000000000E-01,
 BUA     =    0.                    ,
 BUB     =    0.                    ,
 RUMAX   =    0.                    ,
 BUDV    =    0.                    ,
$END
```

```
$N
 NMAT    =        22,
 NN      =        -1,
$END
         ***** 9404 BUILD UP EOS    *****


$DAT
 IEXP    =         5,
 IBRN    =         1,
 IVIS    =         0,
 VFACT   =    2.5000000000000E+00,
 RHOO    =    1.8440000000000E+00,
 PO      =    1.0000000000000E-06,
 TO      =    3.0000000000000E+02,
 EO      =    0.                  ,
 UO      =    0.                  ,
 SOL     =    2.7150000000000E-01,   2.5760000000000E+00,
              1.0000000000000E-01,   0.                  ,
              0.                  ,  -8.6661849555200E+00,
             -5.8313782208900E+01,   -6.9716341085000E+01,
             -8.2009910278300E+00,   2.0719556900800E+01,
              6.7470000000000E-01,   4.0000000000000E-01,
              5.4229935000000E-01,   5.0000000000000E-05,
              0.                  ,  0.                  ,
              3.0000000000000E+02,   1.0000000000000E-06,
              0.                  ,  0.                  ,
              0.                  ,  1.0000000000000E-06,
              0.                  ,
 WO      =    1.0000000000000E+00,
 Z       =    0.                  ,
 E       =    0.                  ,
 VCJ     =    4.1469950000000E-01,
 DCJ     =    4.1469950000000E-01,
 BCJUP   =    0.                  ,
 NDWDT   =         0,
 BPCJ    =    0.                  ,
 AMINP   =    0.                  ,
 DWDT    =    0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
              0.                  ,   0.                  ,
 GAS     =   -3.9513022262000E+00,   -3.2500000000000E+00,
              0.                  ,   0.                  ,
              0.                  ,  -1.6427052459600E+00,
              5.1809393382100E-01,   8.7301259389500E-02,
              6.5604492690900E-03,   1.8255953940800E-04,
              0.                  ,  -1.1669894169900E+00,
              0.                  ,   0.                  ,
              0.                  ,   5.0000000000000E-01,
              1.0000000000000E-01,
 BUA     =    2.6800000000000E+00,
 BUB     =    1.3900000000000E+00,
 BUMAX   =    3.7000000000000E+00,
 BUDV    =    8.8000000000000E-01,
$END
```

```
$N
 NMAT    =        23,
 NN      =        -1,
$END
          ***** 9404 GAMMA LAW       *****


$DAT
 IEXP    =         1,
 IBRN    =         2,
 IVIS    =         0,
 VFACT   =    2.5000000000000E+00,
 RHOO    =    1.8440000000000E+00,
 PO      =    1.0000000000000E-06,
 TO      =    3.0000000003000E+02,
 EO      =    0.                    ,
 UO      =    0.                    ,
 SML     =    2.7150000000300E-01,    2.5760000000000E+00,
              1.0000000000000E-01,    0.                    ,
              0.                    ,   -8.6661849555200E+00,
             -5.8313782208900E+01,   -6.9715341085000E+01,
             -8.2009910278300E+00,    2.0719556900800E+01,
              6.7470000000000E-01,    4.0000000000000E-01,
              5.4229935000000E-01,    5.0000000000300E-05,
              0.                    ,   0.                    ,
              3.0000000000000E+02,    1.0000000000000E-06,
              0.                    ,   0.                    ,
              0.                    ,   1.0000000000000E-06,
              0.                    ,
 WO      =    1.0000000000000E+00,
 Z       =    0.                    ,
 E       =    0.                    ,
 VCJ     =    6.8000000000000E-01,
 DCJ     =    8.8000000000000E-01,
 BCJUP   =    0.                    ,
 NDWDT   =         0,
 BPCJ    =    0.                    ,
 AMINP   =    0.                    ,
 DWDT    =    0.                    ,   0.                    ,
              0.                    ,   0.                    ,
              0.                    ,   0.                    ,
              0.                    ,   0.                    ,
              0.                    ,   0.                    ,
              0.                    ,   0.                    ,
              0.                    ,   0.                    ,
              0.                    ,   0.                    ,
              0.                    ,   0.                    ,
              0.                    ,   0.                    ,
 GAS     =   -3.9513022262000E+00,   -3.2500000000000E+00,
              0.                    ,   0.                    ,
              0.                    ,   -1.6427052459600E+00,
              5.1809393382100E-01,    8.7301259389500E-02,
              6.5604492690900E-03,    1.8255953940800E-04,
              0.                    ,   -1.1669884169900E+00,
              0.                    ,   0.                    ,
              0.                    ,   5.0000000000000E-01,
              1.0000000000000E-01,
 BUA     =    0.                    ,
 BUB     =    0.                    ,
 BUMAX   =    0.                    ,
 BUDV    =    0.                    ,
$END
```

```
$N
 NMAT   =        24,
 NN     =        -1,
$END
      *****  9404 FOREST FIRE     *****

$DAT
 IEXP   =         1,
 IBRN   =         4,
 IVIS   =         2,
 VFACT  =    2.0000000000000E-03,
 RHOO   =    1.8440000000000E+00,
 PO     =    1.0000000000000E-06,
 TO     =    3.0000000000000E+02,
 EO     =    0.                    ,
 UO     =    0.                    ,
 SOL    =    2.4230000000000E-01,    1.8830000000000E+00,
             1.0000000000000E-02,    0.                   ,
             0.                    ,   -9.0418722204200E+00,
            -7.1318525243500E+01,    -1.2520497936000E+02,
            -9.2042417760300E+01,    -2.2189382572700E+01,
             6.7500000000000E-01,     4.0000000000000E-01,
             5.4229934924100E-01,     5.0000000000000E-05,
             0.                    ,   0.                   ,
             3.0000000000000E+02,     1.0000000000000E-06,
             0.                    ,   0.                   ,
             0.                    ,   0.                   ,
             0.                    ,
 WO     =    1.0000000000000E+00,
 Z      =    0.                    ,
 E      =    0.                    ,
 VCJ    =    8.8800000000000E-01,
 DCJ    =    0.                    ,
 RCJUP  =    0.                    ,
 NDWDT  =        14,
 RPCJ   =    3.6300000000000E-01,
 AMINP  =    1.5000000000000E-02,
 DWDT   =    2.5277953727000E+10,    -6.9876099170000E+10,
             8.6704208069000E+10,    -6.3781135352000E+10,
             3.0950369616000E+10,    -1.0433258901000E+10,
             2.5068548091000E+09,    -4.3377143285000E+08,
             5.4017707404000E+07,    -4.7962436917000E+06,
             2.9889932207000E+05,    -1.2887959724000E+04,
             4.0524452315000E+02,    -8.3979132644000E+00,
             0.                    ,   0.                   ,
             0.                    ,   0.                   ,
             0.                    ,   0.                   ,
 GAS    =   -3.5390625996400E+00,    -2.5773759039300E+00,
             2.6007542333200E-01,     1.3908357850800E-02,
            -1.1396302407500E-02,    -1.6191304113300E+00,
             5.2151853419200E-01,     6.7750659410700E-02,
             4.2652426469100E-03,     1.0467999990200E-04,
             7.3642291979000E+00,    -4.9365822238900E-01,
             2.9235306096100E-02,     3.3027740221900E-02,
            -1.1453249820600E-02,     5.0000000000000E-01,
             1.0000000000000E-01,
 BUA    =    0.                    ,
 BUB    =    0.                    ,
 BUMAX  =    0.                    ,
 BUDV   =    0.                    ,
$END
```

```
$N
 NMAT    =        25,
 NN      =        -1,
$END
          ***** TATB/WAX FF F(P)     *****


$DAT
 IEXP    =         1,
 IBRN    =         4,
 IVIS    =         1,
 VFACT   =    4.0000000000000E-01,
 RHOO    =    1.7410000000000E+00,
 PO      =    1.0000000000000E-06,
 TO      =    3.0000000000000E+02,
 EO      =    0.                    ,
 UO      =    0.                    ,
 SOL     =    2.6200000000000E-01,    1.8460000000000E+00,
              1.0000000000000E-02,    0.                   ,
              0.                   , -1.0565561479500E+01,
             -8.8519912048700E+01,   -1.7580617026200E+02,
             -1.4821742233500E+02,   -4.2691241225500E+01,
              1.7000000000000E+00,    1.0000000000000E+00,
              5.7438253877100E-01,    5.0000000000000E-05,
              0.                   ,  0.                   ,
              3.0000000000000E+02,    1.0000000000000E-06,
              0.                   ,  0.                   ,
              0.                   ,  1.0000000000000E-06,
              0.                   ,
 WO      =    1.0000000000000E+00,
 Z       =    0.                    ,
 E       =    0.                    ,
 VCJ     =    0.                    ,
 DCJ     =    0.                    ,
 BCJUP   =    0.                    ,
 NDWDT   =        15,
 BPCJ    =    2.4200000000000E-01,
 AMINP   =    5.0000000000000E-02,
 DWDT    =    2.1074823834300E+15,   -4.0485613115500E+15,
              3.5604013860000E+15,   -1.8095456595000E+15,
              6.8538310052000E+14,   -1.7708730387300E+14,
              3.3749845396400E+13,   -4.8166840092100E+12,
              5.1695074669000E+11,   -4.1491881910200E+10,
              2.4497203379100E+09,   -1.0306137019700E+08,
              2.9147295142500E+06,   -4.9191520774900E+04,
              3.4692852517900E+02,    0.                   ,
              0.                   ,  0.                   ,
              0.                   ,  0.                   ,
 GAS     =   -3.8151151160600E+00,   -2.6820304590800E+00,
              2.6707281671500E-01,    1.1008177275600E-01,
             -4.2627029473100E-02,   -1.5324690993000E+00,
              5.6368029118800E-01,    1.1099121788600E-01,
              1.1097910232600E-02,    4.3719078163500E-04,
              7.2050716427100E+00,   -4.7824523434400E-01,
              6.0919683634800E-02,    7.4133402313400E-03,
             -5.0885279490900E-03,    5.0000000000000E-01,
              1.0000000000000E-01,
 BUA     =    0.                    ,
 BUB     =    0.                    ,
 BUMAX   =    0.                    ,
 BUDV    =    0.                    ,
$END
```

```
$N
 NMAT    =        26,
 NN      =        -1,
$END
          ***** X0290 FF PCJ=.285    *****


$DAT
 IEXP    =         1,
 IRRN    =         4,
 IVIS    =         0,
 VFACT   =    2.0000000000000E+00,
 RHOO    =    1.8940000000000E+00,
 PO      =    0.                  ,
 TO      =    0.                  ,
 EO      =    0.                  ,
 UO      =    0.                  ,
 SOL     =    2.4000000000000E-01,    2.0500000000000E+00,
              0.                  ,    0.                  ,
              0.                  ,   -2.3014158556000E+01,
             -1.3631901377800E+02,   -2.3506821666100E+02,
             -1.7104959098300E+02,   -4.2263550556900E+01,
              1.5000000000000E+00,    3.0000000000000E-01,
              5.2798310454100E-01,    5.0000000000000E-05,
              0.                  ,    0.                  ,
              3.0000000000000E+02,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,
 WO      =    1.0000000000000E+00,
 Z       =    0.                  ,
 E       =    0.                  ,
 VCJ     =    3.9423000000000E-01,
 DCJ     =    0.                  ,
 RCJUP   =    0.                  ,
 NDWDT   =        15,
 RPCJ    =    2.8500000000000E-01,
 AMINP   =    5.5000000000000E-02,
 DWDT    =    8.1425481008000E+13,   -1.9413898714000E+14,
              2.1097494446000E+14,   -1.3836158944000E+14,
              6.1110150327000E+13,   -1.9205772744000E+13,
              4.4248348854000E+12,   -7.5817519329000E+11,
              9.6978690159000E+10,   -9.2043893492000E+09,
              6.3734890585000E+08,   -3.1181988011000E+07,
              1.5170082035000E+06,   -1.9660891926000E+04,
              1.6223658470000E+02,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
 GAS     =   -3.8782854115900E+00,   -2.6903229723100E+00,
              2.2207418495100E-01,    7.4248212800000E-02,
             -3.4281943072700E-02,   -1.5889961537700E+00,
              5.3489544838500E-01,    9.4282425112400E-02,
              8.2564345992400E-03,    2.8935792258200E-04,
              7.0674029264900E+00,   -5.6700324443000E-01,
              5.1794158609500E-02,    9.8485394639500E-03,
             -1.0921841974800E-02,    5.0000000000000E-01,
              1.0000000000000E-01,
 RUA     =    0.                  ,
 RUB     =    0.                  ,
 RUMAX   =    0.                  ,
 RUDV    =    0.                  ,
$END
```

```
$N
 NMAT    =        27,
 NN      =        -1,
$END
          ***** NQ/ESTANE 95/5 FF(T) *****


$DAT
 IEXP    =         1,
 IBRN    =         4,
 IVIS    =         1,
 VFACT   =    2.5000000000000E+00,
 RHOO    =    1.6990000000000E+00,
 PO      =    0.                  ,
 TO      =    3.0000000000000E+02,
 EO      =    0.                  ,
 UO      =    0.                  ,
 SOL     =    3.0000000000000E-01,    1.7950000000000E+00,
              0.                  ,    0.                  ,
              0.                  ,   -4.3375662728300E+00,
             -5.2981710589500E+01,   -1.0134141654400E+02,
             -8.1576457053800E+01,   -2.1688340014100E+01,
              1.5000000000000E+00,    1.0000000000000E+00,
              5.8858151000000E-01,    5.0000000000000E-05,
              0.                  ,    0.                  ,
              3.0000000000000E+02,    1.0000000000000E-06,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,
 WO      =    1.0000000000000E+00,
 Z       =    0.                  ,
 E       =    0.                  ,
 VCJ     =    0.                  ,
 DCJ     =    0.                  ,
 BCJUP   =    0.                  ,
 NDWDT   =        15,
 BPCJ    =    1.3965931925800E+03,
 AMINP   =    3.9413000365800E+02,
 DWDT    =   -2.4754151108200E-37,    2.9718825932700E-33,
             -1.6403011725300E-29,    5.5162577515100E-26,
             -1.2626800047100E-22,    2.0810584469500E-19,
             -2.5467895398800E-16,    2.3512495264500E-13,
             -1.6458549154900E-10,    8.6951979083100E-08,
             -3.4143685421200E-05,    9.6694517066900E-03,
             -1.8688014733600E+00,    2.2101444421200E+02,
             -1.2115464430700E+04,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
 GAS     =   -3.7813223223600E+00,   -2.8659072289500E+00,
              4.5780376665900E-01,   -2.1393476004800E-01,
             -3.8759650139800E-01,   -1.5813814217000E+00,
              5.3353834411400E-01,    9.1038624589100E-02,
              7.3248274107000E-03,    2.3436649822400E-04,
              6.7027481505400E+00,   -6.6694075746100E-01,
              1.7172154149600E-01,   -2.3654570859100E-01,
             -3.8360574585200E-01,    5.0000000000000E-01,
              1.0000000000000E-01,
 BUA     =    0.                  ,
 BUB     =    0.                  ,
 BUMAX   =    0.                  ,
 BUDV    =    0.                  ,
$END
```

```
$N
 NMAT    =        30,
 NN      =        -1,
$END
          ***** NO FF RH ZERO ORDER  *****


$DAT
 IEXP    =         1,
 IBRN    =         4,
 IVIS    =         1,
 VFACT   =    2.5000000000000E+00,
 RHOO    =    1.6990000000000E+00,
 PO      =    0.                  ,
 TO      =    3.0000000000000E+02,
 EO      =    0.                  ,
 UO      =    0.                  ,
 SOL     =    3.0000000000000E-01,    1.7950000000000E+00,
              0.                  ,    0.                  ,
              0.                  ,   -4.3375662728300E+00,
             -5.2981710589500E+01,   -1.0134141654400E+02,
             -8.1576457053800E+01,   -2.1688340014100E+01,
              1.5000000000000E+00,    1.0000000000000E+00,
              5.9858151000000E-01,    5.0000000000000E-05,
              0.                  ,    0.                  ,
              3.0000000000000E+02,    1.0000000000000E-06,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,
 WO      =    1.0000000000000E+00,
 Y       =    0.                  ,
 E       =    0.                  ,
 VCJ     =    0.                  ,
 DCJ     =    0.                  ,
 BCJUP   =    0.                  ,
 NDWDT   =        15,
 BPCJ    =    2.8500000000000E-01,
 AMINP   =    9.0000000000000E-02,
 DWDT    =    1.0493710061000E+13,   -2.4403909027000E+13,
              2.5848703251000E+13,   -1.6509273785000E+13,
              7.0926386979000E+12,   -2.1655438309000E+12,
              4.8379711632000E+11,   -8.0196999294000E+10,
              9.8904508407000E+09,   -9.0036142748000E+08,
              5.9260988094000E+07,   -2.7058239629000E+06,
              7.8400413699000E+04,   -1.0435423528000E+03,
             -1.4056835920000E+01,    0.                  ,
              0.                  ,    0.                  ,
              0.                  ,    0.                  ,
 GAS     =   -3.7813223223600E+00,   -2.8669072289500E+00,
              4.5780376665900E-01,   -2.1393476004800E-01,
             -3.8759650139800E-01,   -1.5813814217000E+00,
              5.3353834411400E-01,    9.1038624589100E-02,
              7.3248274107000E-03,    2.3436649822400E-04,
              6.7027481505400E+00,   -6.6694075746100E-01,
              1.7172154149600E-01,   -2.3654570859100E-01,
             -3.8360574585200E-01,    5.0000000000000E-01,
              1.0000000000000E-01,
 BUA     =    0.                  ,
 BUB     =    0.                  ,
 BUMAX   =    0.                  ,
 BUDV    =    0.                  ,
$END
```

```
$N
 NMAT   =        31,
 NN     =        -1,
$END
         *****  TNT                    *****


$DAT
 IEXP   =         1,
 ISRN   =         1,
 IVIS   =         0,
 VFACT  =    2.0000000000000E+00,
 RHOO   =    1.6400000000000E+00,
 PO     =    1.0000000000000E-06,
 TO     =    3.0000000000000E+02,
 EO     =    0.                    ,
 UO     =    0.                    ,
 SOL    =    3.0330000000000E-01,    1.3660000000000E+00,
             1.0000000000000E-03,    0.                    ,
             0.                    ,    1.1487924489200E+01,
             2.9423815334900E+01,    5.1407881602000E+01,
             3.6666803808000E+01,    1.0775309358200E+01,
             1.7300000000000E+00,    2.9300000000000E-01,
             6.0975609760000E-01,    5.0000000000000E-05,
             0.                    ,    0.                    ,
             3.0000000000000E+02,    1.0000000000000E-06,
             0.                    ,    0.                    ,
             0.                    ,    1.0000000000000E-06,
             0.                    ,
 WO     =    1.0000000000000E+00,
 Z      =    0.                    ,
 E      =    0.                    ,
 VCJ    =    4.6300000000000E-01,
 DCJ    =    4.6300000000000E-01,
 BCJUP  =    0.                    ,
 NDWDT  =         0,
 BPCJ   =    0.                    ,
 AMINP  =    0.                    ,
 DWDT   =    0.                    ,    0.                    ,
             0.                    ,    0.                    ,
             0.                    ,    0.                    ,
             0.                    ,    0.                    ,
             0.                    ,    0.                    ,
             0.                    ,    0.                    ,
             0.                    ,    0.                    ,
             0.                    ,    0.                    ,
             0.                    ,    0.                    ,
             0.                    ,    0.                    ,
 GAS    =   -4.0927913585100E+00,   -3.1600000000000E+00,
             0.                    ,    0.                    ,
             0.                    ,   -1.4017487387500E+00,
             4.6320457097100E-01,    8.2694800461400E-02,
             6.7200941511000E-03,    2.0718222636500E-04,
             0.                    ,   -9.9000000000000E-01,
             0.                    ,    0.                    ,
             0.                    ,    5.0000000000000E-01,
             1.0000000000000E-01,
 BUA    =    0.                    ,
 BUB    =    0.                    ,
 BUMAX  =    0.                    ,
 BUDV   =    0.                    ,
$END
```

B. Using the SESAME Option in HYDROX (by G. I. Kerley)

Specify a SESAME EOS in NAMELIST SU, by setting IEOS = 4 and MAT equal to the material number. In NAMELIST ESC, specify the parameters for spall, viscosity, and elastic-plastic flow, as with other EOS options. In order to use special options available with the SESAME tables, specify the parameters discussed below.

1. Initial State Calculation. In NAMELIST ESC,

ROW = initial density in g/cm^3

TO = initial temperature in K

ZI = initial internal energy ($Mbar\text{-}cm^3/g$)

If ROW is not input, the code will obtain this quantity from the SESAME library. An input value will override the SESAME number. Parameters TO and ZI default to zero.

If the user specifies TO $\neq$ 0 and if ZI = 0, the code will calculate ZI from ROW and TO. This feature is especially useful when the material is a gas, but it can be used for solids and liquids as well.

2. Density and Energy Scaling. In NAMELIST ESC,

SR = density scale factor (default = 1)

ES = energy shift in $Mbar\text{-}cm^3/g$ (default = 0)

Using these parameters, the EOS is scaled according to the following relations.

$$\begin{aligned} P(\rho,E) &= P_{TAB}(\rho_T, E_T) \quad , \\ \rho_T &= SR^* \rho \quad , \\ E_T &= (E + ES)/SR \quad , \end{aligned} \tag{1}$$

where P, ρ, and E are the pressure, density, and energy variables used by the code, and $P_{TAB}(\rho_T, E_T)$ is the tabular EOS.

The parameter SR is useful for treating isotopic mixtures. If A_T is the atomic weight for the EOS table, an EOS for an atomic weight A is obtained by setting

$$SR = A_T/A \quad . \tag{2}$$

For example, set SR = 2 to scale the SESAME D_2 EOS, #5263, to H_2. Similarly, set SR = .80 to obtain an EOS for a 50:50 DT mixture.

The parameter ES can be used to change the energy zero of the table. It is intended for use primarily with the "ramp" option, discussed below.

3. Foams and Phase Transitions. In NAMELIST ESC,

A1, A2, A3 = ramp parameters (default = 0)

ES = energy shift in Mbar-cm^3/g (default = 0)

IRV = reversible/irreversible flag (default = 0)

EM = "melt" energy in Mbar-cm^3/g (default = 1000)

For treatment of foams and certain types of phase transitions, it is possible to modify the SESAME EOS by adding a "ramp" which describes the behavior of the material at low stress levels.

The material starts out in either a porous state or low-density phase. The EOS as a function of the density ρ is given by

$$P = A_1(\rho/\rho_0 - 1) \quad , \tag{3}$$

where ρ_0 is the initial density (ROW) and A_1 is the bulk modulus in Mbar. A_1 can be computed from

$$A_1 = 0.01\rho_0 C_0^2 \tag{4}$$

where C_0 is the bulk sound speed in km/s. If $A_1 = 0$, no ramp calculation is performed.

At some pressure P_i, the material will begin to "crush," or transform to the high-density phase which is described by the SESAME EOS. The EOS of the crush curve is

$$P = A_2(\rho/\rho_0 - A_3) \quad . \tag{5}$$

(If $A_2 = 0$, there is no crush region and Eq. (3) is continued on until it crosses the SESAME hydrostat.) A_2 is related to the transition pressure by

$$A_2 = \frac{P_i A_1}{P_i + A_1(1 - A_3)} \quad \text{(Mbar)}. \tag{6}$$

The transition pressure for foams is usually rather small (<1 kbar). For a phase transition, P_i must be obtained from experiment. The parameter A_3 can be adjusted to give the correct slope of the crush curve. In the absence of data, the default value ($A_3 = 0$) should give acceptable results.

At some pressure P_f, the ramp crosses the SESAME hydrostat. At that point, the cell is said to be "crushed." Subsequently, the material may behave either reversibly (follow the ramp on expansion) or irreversibly (stay in the high-density phase on expansion). Foams are normally irreversible, but phase transitions may be either. The behavior is controlled by setting

$$\text{IRV} = \begin{matrix} 1 & \text{reversible,} \\ 0 & \text{irreversible,} \end{matrix} \tag{7}$$

where the default is IRV = 0. In HYDROX, the material will also behave irreversibly if it melts; i.e., if the melt energy EM is exceeded. EM depends upon the path and must be treated carefully. The default value (EM = 1000) is sufficiently high that "melting" will not occur in most cases of interest.

For foams, the energy shift ES should be set to zero. For phase transitions, set

$$\text{ES} = -\Delta E \text{ (initial} \rightarrow \text{final)} \quad , \tag{8}$$

where ΔE is the energy required to transform the low-density phase to the high-density phase. Hence there are two cases. If the initial phase is stable, ES is negative. If the initial phase is metastable, ES is positive.

4. Interpolation Option. In NAMELIST INP, set

IFN = 0 rational function algorithm,

IFN = 1 bilinear algorithm,

where the default is IFN = 0. The rational function option is the more accurate interpolation scheme. The bilinear scheme is faster and is sufficiently accurate for some applications.

5. Table of SESAME Materials in SES2L

SHORT SUMMARY FOR VERSION 67 OF SESAME LIBRARY FILE SES2L
DATED 91280 FOR 45 MATERIALS

NUMBER	MATERIAL	ZBAR	ABAR	RO	TABLES
1540	URANIUM	92.0	238.0	19.0	101 201 301
2020	BERYLLIUM	4.0	9.0	1.8	101 102 201 301
2021	BERYLLIUM	4.0	9.0	1.9	101 201 301
2140	IRON	26.0	55.9	7.9	101 201 301
2144	IRON	26.0	55.9	7.9	101 102 201 301
2145	IRON - REACTOR SAFET	26.0	55.9	7.9	101 102 201 301 401
2200	LITHIUM	3.0	6.9	.5	101 201 301
2445	SODIUM	11.0	23.0	1.0	101 102 201 301
2446	SODIUM	11.0	23.0	1.0	101 102 201 301
2448	SODIUM	11.0	23.0	1.0	101 201 301 401
2700	GOLD	79.0	197.0	19.3	101 102 201 301
2701	GOLD	79.0	197.0	19.3	101 201 301
2980	MOLYBDENUM	42.0	95.9	10.2	101 201 301
3100	NICKEL	28.0	58.7	8.9	101 201 301
3200	LEAD	82.0	207.2	11.3	101 102 201 301
3330	COPPER	29.0	63.5	8.9	101 201 301
3541	TUNGSTEN	74.0	183.9	19.2	101 201 301
3710	ALUMINUM	13.0	27.0	2.7	101 201 301
3730	PLATINUM	78.0	195.1	21.4	101 201 301
4100	BRASS	29.8	65.3	8.5	101 102 201 301
4270	STAINLESS STEEL	25.8	55.4	7.9	101 201 301
4271	STEEL	26.0	55.8	7.9	101 201 301
5170	ARGON	18.0	39.9	1.5	101 102 201 301
5180	KRYPTON	36.0	83.8	2.5	101 102 201 301
5263	DEUTERIUM	1.0	2.0	.2	101 102 201 301 303
5410	NEON	10.0	20.2	1.4	101 201 301
5500	METHANE	2.0	3.2	.5	101 102 201 301 401
5501	METHANE	2.0	3.2	.5	101 102 201 301 401
5760	HELIUM	2.0	4.0	.2	101 201 301
7081	BORON CARBIDE - REAC	5.2	10.4	2.5	101 201 301 401
7111	NEVADA ALLUVIUM	9.4	19.8	2.4	101 201 301
7150	WATER	3.3	6.0	1.0	101 201 301
7151	STEAM	3.3	6.0	1.0	101 201 301
7170	POLYETHYLENE	2.7	4.7	.9	101 201 301
7240	LITHIUM DEUTERIDE	2.0	4.0	.8	101 201 301
7370	LITHIUM HYDRIDE	2.0	3.5	.7	101 201 301
7380	QUARTZ	10.0	20.0	2.2	101 201 301
7390	WESTERLY GRANITE	10.3	20.7	2.6	101 201 301
7410	ALUMINA	10.0	20.4	4.0	101 201 301
7432	URANIUM DIOXIDE	36.0	90.0	11.0	101 201 301 401
7520	MICA	6.9	13.5	2.7	101 201 301
7560	POLYURETHANE	3.8	7.0	1.3	101 201 301

7590	POLYSTYRENE	3.5	6.5	1.0	101	201	301
7830	DIAMOND	6.0	12.0	3.5	101	201	301
8180	HIGH EXPLOSIVE	5.6	11.0	1.8	101	201	301

NOTES.

TABLES 100-199	CONTAIN HOLLERITH DATA
TABLES 201	CONTAIN BASIC DATA
TABLES 301	CONTAIN TOTAL EOS DATA
TABLES 303	CONTAIN ION EOS DATA
TABLES 401	CONTAIN VAPORIZATION DATA

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