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Informal Report

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Numerical Modeling of Insensitive High-Explosive Initiators

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Numerical Modeling of Insensitive High-Explosive Initiators

Charles L. Mader

NUMERICAL MODELING OF INSENSITIVE HIGH-EXPLOSIVE INITIATORS

by

Charles L. Mader

ABSTRACT

The initiation of propagating detonation in PBX-9404, PBX-9502, and X0219 by hemispherical initiators of PBX-9404, 1.8 g/cm^3 TATB, and X0351 is described numerically, using the two-dimensional Lagrangian code 2DL and the Forest Fire rate to describe the heterogeneous explosive shock initiation process.

I. INTRODUCTION

The initiation of propagating, diverging detonation is usually accomplished by small conventional initiators; however, as the explosive to be initiated becomes more shock insensitive, the initiators must have larger diameters (>2.5 cm) to be effective.

Travis[1] has used the I^{2}C camera to examine the nature of the diverging detonation waves formed in PBX-9404 (94/3/3 HMX/nitrocellulose/Tris-β-chloroethyl phosphate), X0290 or PBX-9502 (95/5 TATB/Kel-F at 1.894 g/cm^3), and X0219 (90/10 TATB/Kel F at 1.914 g/cm^3) by hemispherical initiators. The geometries of the initiators were (1) a 6.35-mm-radius hemisphere of PBX-9407 (94/6 RDX/Exon at 1.61 g/cm^3) surrounded by a 6.35-mm-thick hemisphere of PBX-9404, (2) a 6.35-mm-radius hemisphere of 1.7-g/cm^3 TATB surrounded by a 19.05-mm-thick hemisphere of 1.8-g/cm^3 TATB, or (3) a 16-mm-radius hemisphere of X0351 (15/5/80 HMX/Kel-F/TATB at 1.89 g/cm^3).

We have numerically examined systems with similar geometries by use of the hydrodynamic code 2DL[2] and the Forest Fire rate[2] to describe the shock initiation process.

II. NUMERICAL MODELING

The two-dimensional reactive Lagrangian hydrodynamic code 2DL[2] was used to describe the reactive fluid dynamics. The Forest Fire[2] description of heterogeneous shock initiation was used to describe the explosive burn. The HOM equation of state and Forest Fire rate constants for PBX-9502, PBX-9404, and X0219 were identical to those described in Ref. 2. The Pop plots are shown in Fig. 1

and the Forest Fire rates in Fig. 2. The BKW detonation product equation-of-state constants for X0351 and for 1.7- and 1.8-g/cm^3 TATB are given in Tables I, II, and III.

The calculations were done in cylindrical geometry with Lucite confinement rather than the air confinement present in the experimental study. The Lucite confinement prevents the mesh distortion that can be fatal to Lagrangian calculations.

The central 6.35-mm region of the detonator is initially exploded, which initiates the remaining explosive in the detonator using a C-J volume burn. For any given mesh size and time step, the viscosity must be adjusted to give a peak pressure at the detonation front near the effective C-J pressure. The parameters used are as follows.

Calculation		Mesh Size	Time Step	Viscosity
Initiator	Acceptor	(cm)	(μs)	Coefficient
PBX-9407/PBX-9404	PBX-9404	0.05	0.02	4.0
PBX-9407/PBX-9404	PBX-9502	0.05	0.02	5.0
PBX-9407/PBX-9404	X0219	0.05	0.02	4.2
1.7 TATB/1.8 TATB	PBX-9502	0.1	0.02	5.0
X0351	PBX-9502	0.1	0.02	5.0

The pressure and mass fraction contours are shown for a PBX-9404 hemisphere initiating PBX-9404 in Fig. 3, PBX-9502 (X0290) in Fig. 4, and X0219 in Fig. 5. The experimental[1] and calculated position of the leading wave as a function of distance from the origin is shown in Fig. 6.

The burn can become unstable when it turns a corner. The instability is apparently numerical because it can be eliminated by using an average of nearby cell pressures for the Forest Fire burn rather than the individual cell pressure.

The pressure and mass fraction contours are shown in Fig. 7 for the 1.8-g/cm^3 TATB hemisphere initiating PBX-9502. Very little undecomposed explosive was observed experimentally, in agreement with the calculated results. The contours are shown in Fig. 8 for an X0351 hemisphere initiating PBX-9502. The experimental and calculated regions of partially decomposed PBX-9502 are shown in Fig. 9.

III. CONCLUSIONS

The initiation of propagating detonation in sensitive (PBX-9404) and insensitive (PBX-9502 and X0219) explosives by hemispherical initiators can be described numerically using the two-dimensional Lagrangian code 2DL and the Forest Fire rate. Large regions of partially decomposed explosive occur even when insensitive explosives are initiated by large initiators.

REFERENCES

1. James R. Travis, Los Alamos Scientific Laboratory, personal communication.

2. Charles L. Mader, Numerical Modeling of Detonations (University of California Press, Berkeley, 1979).

TABLE I

BKW EQUATION OF STATE FOR X0351

```
A FORTRAN BKW CALCULATION FOR THE EXPLOSIVE
X0351  15/5/80 HMX/KELF/TATB

THE NUMBER OF ELEMENTS IS      6

THE NUMBER OF GAS SPECIES IS    18

THE NUMBER OF SOLID SPECIES IS     1

THE BKW EQUATION OF STATE PARAMETERS ARE
 ALPHA= 5.00000000000E-01 BETA= 9.58500000000E-02 THETA= 4.00000000000E+02 KAPPA= 1.26847111054E+01

THE COMPOSITION OF THE EXPLOSIVE IS
     6.93050000000E+00 MOLES OF   C
     7.30712000000E+00 MOLES OF   H
     7.30712000000E+00 MOLES OF   N
     7.30712000000E+00 MOLES OF   O
     4.15410000000E-01 MOLES OF   F
     1.38470000000E-01 MOLES OF   CL

THE DENSITY OF THE EXPLOSIVE IS  1.89000000000E+00, GRAMS/CC

THE MOLECULAR WEIGHT IS  3.22620000000E+02 GRAMS

THE HEAT OF FORMATION AT 0 DEG K IS -2.99800000000E+04 CALORIES PER FORMULA WEIGHT

THE SOLID (COWAN) EQUATION OF STATE PARAMETERS    VO, AS, BS, CS, DS, ES,    A1, A2, C1, C2, C3, ATOMIC WT

SOL C   4.44444444444E-01  8.30935837268E-01  -1.39381809219E+00  6.72569716021E-01  -1.13537262508E-01  6.49155882007E-1
       -2.26705345948E-01  1.20516569525E-01   8.31600000000E-02 -1.75590000000E-01   1.55310000000E-01  1.20100000000E+1
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TABLE I (cont)

THE COMPUTED CJ PRESSURE IS 2.94802491866E-01 MEGABARS

THE COMPUTED DETONATION VELOCITY IS 7.80963238225E-01 CM/MICROSECOND

THE COMPUTED CJ TEMPERATURE IS 2.17522460605E+03 DEGREES KELVIN

THE COMPUTED CJ VOLUME 3.93785857949E-01 CC/GM OF EXPLOSIVE

THE COMPUTED GAMMA IS 2.91013575863E+00

THE VOLUME OF THE GAS IS 1.17736418375E+01 CC/MOLE OF GAS AND THERE ARE 9.28201924192E+00 MOLES OF GAS

SOLID	VOLUME IN CC/GM
SOL C	2.98076862285E-01

THE C-J COMPOSITION OF THE DETONATION PRODUCTS AND THE INPUT COEFFICIENTS TO THE THERMODYNAMIC FITS FOR EACH SPECIE

SPECIE	NO OF MOLES	COEFFICIENTS A,B,C,D,E, THE INTEGRATION CONSTANT, HEAT OF FORMATION IN CAL/MOLE,COVOLUME				
HF	9.84775860361E-03	4.00007100000E+01	1.14458200000E-02	-2.21043000000E-06	1.68170500000E-10	0.
		1.17900480281E+03	-6.42000000000E+04	3.89000000000E+02		
CF4	1.01380532789E-01	5.56800600000E+01	3.56363400000E-02	-6.88817200000E-06	5.16953400000E-10	0.
		2.03728882709E+02	-2.18000000000E+05	1.33000000000E+03		
F2	1.72885498353E-08	4.63724900000E+01	1.39582500000E-02	-2.80475800000E-06	2.15833800000E-10	0.
		9.56070057282E+02	0.	3.87000000000E+02		
H2O	3.64825197617E+00	4.25804200000E+01	1.48080500000E-02	-2.63918100000E-06	1.92045300000E-10	0.
		1.34282835158E+03	-5.71070000000E+04	2.50000000000E+02		
H2	5.14255002734E-06	2.97034700000E+01	1.14382900000E-02	-2.20122200000E-06	1.67776100000E-10	0.
		1.17588815385E+03	0.	1.80000000000E+02		
O2	6.87392520397E-08	4.70309000000E+01	1.28714700000E-02	-2.50021700000E-06	1.90157000000E-10	0.
		1.03537847388E+03	0.	3.50000000000E+02		
CO2	1.82511983588E+00	4.74811200000E+01	1.95446300000E-02	-3.72129800000E-06	2.77030000000E-10	0.
		7.46200988750E+02	-9.39680000000E+04	6.00000000000E+02		
CO	8.62237904089E-03	4.53308200000E+01	1.23816100000E-02	-2.41640300000E-06	1.82818100000E-10	0.
		1.12158830990E+03	-2.72010000000E+04	3.90000000000E+02		
NH3	6.27898564309E-05	4.20181600000E+01	1.91168200000E-02	-3.16433000000E-06	2.19780100000E-10	0.
		1.20898121615E+03	-9.36800000000E+03	4.76000000000E+02		
H	1.03040578311E-09	2.63911000000E+01	8.12137200000E-03	-1.69074000000E-06	1.31682300000E-10	0.
		7.94631617188E+02	5.16190000000E+04	7.60000000000E+01		
NO	5.79518662335E-06	4.84149800000E+01	1.26938600000E-02	-2.49460000000E-06	1.89321300000E-10	0.
		1.20924970573E+03	2.14770000000E+04	3.86000000000E+02		
N2	3.65352570748E+00	4.39234000000E+01	1.22250100000E-02	-2.37900500000E-06	1.79832200000E-10	0.
		1.13916134898E+03	0.	3.80000000000E+02		

TABLE I (cont)

OH	1.52263365238E-09	4.24179200000E+01	1.15804700000E-02	-2.22685900000E-06	1.68915500000E-10	0.
		1.18351754427E+03	3.56000000000E+03	4.13000000000E+02		
CH4	1.00287589352E-06	3.87568600000E+01	2.36401300000E-02	-3.70795700000E-06	2.47071400000E-10	0.
		1.04242791146E+03	-1.60000000000E+04	5.28000000000E+02		
COF2	3.88336774269E-08	5.67523300000E+01	2.67670700000E-02	-5.13590100000E-06	3.83331300000E-10	0.
		5.64431820312E+02	-1.50000000000E+05	1.33000000000E+03		
HCL	5.65622325833E-04	4.29366400000E+01	1.18744000000E-02	-2.28640600000E-06	1.72780700000E-10	0.
		1.17374859835E+03	-2.20000000000E+04	6.37000000000E+02		
CCL4	3.43315588584E-02	6.79474000000E+01	3.94821400000E-02	-7.99415600000E-06	6.13624400000E-10	0.
		8.24032489583E+02	-2.55000000000E+04	2.00000000000E+03		
CL2	2.89071520303E-04	5.13210000000E+01	1.43956300000E-02	-2.96388300000E-06	2.34987200000E-10	0.
		9.90222875000E+02	0.	9.56000000000E+02		
SOL C	4.96103465192E+00	-2.46151900000E-01	7.17985500000E-03	-1.29755000000E-06	9.34999500000E-11	0.
		-2.58204389323E+02	0.	0.		

A BKW ISENTROPE THRU BKW CJ PRESSURE FOR
X0351 15/5/80 HMX/KELF/TATB

LN(P)= -3.83124542016E+00 -2.63522252575E+00LNV 2.95483638537E-01LNV*2 5.64219266745E-02LNV*3 -7.56177447579E-02LNV*4

LN(T)= 7.11984046119E+00 -5.49728235763E-01LNV 9.12839783755E-02LNV*2 3.38306262566E-03LNV*3 -3.15977171900E-02LNV*4

LN(E)= -1.58936745306E+00 5.37076400366E-01LNP 9.34679417233E-02LNP*2 8.52247589118E-03LNP*3 3.32705575856E-04LNP*4

THE CONSTANT ADDED TO ENERGIES WAS 1.00000000000E-01

PRESSURE (MBARS)	VOLUME (CC/GM)	TEMPERATURE (DEG K)	ENERGY+C (MB-CC/GM)	GAMMA (-DLNP/DLNV)	PARTICLE VELOCITY
2.94002491866E-01	3.93785866126E-01	2.17522460605E+03	1.19945619785E-01	2.79413469663E+00	1.99727570059E-01
2.06361744306E-01	4.45013525165E-01	2.01819441310E+03	1.07290902121E-01	2.84220249271E+00	2.65965363787E-01
1.44453221014E-01	5.04033129855E-01	1.86222815690E+03	9.70949428620E-02	2.86338385077E+00	3.26547517015E-01
1.01117254710E-01	5.73843525149E-01	1.70872380623E+03	8.86746825563E-02	2.85945463638E+00	3.82553857561E-01
7.07820782970E-02	6.50390017517E-01	1.58178021637E+03	8.21652841296E-02	2.83404345657E+00	4.30716402993E-01
4.95474548079E-02	7.37719874236E-01	1.46864184370E+03	7.69888210702E-02	2.79081317714E+00	4.73520607073E-01
3.46832183855E-02	8.39412354433E-01	1.36410787837E+03	7.27703063997E-02	2.73186379277E+00	5.12304057693E-01
2.42782528559E-02	9.58627327325E-01	1.26746612046E+03	6.93091582159E-02	2.65986759026E+00	5.47488879589E-01
1.69947769991E-02	1.09833118975E+00	1.17858211908E+03	6.64624777422E-02	2.57799559494E+00	5.79466625035E-01
1.18963438994E-02	1.26592216028E+00	1.09545001188E+03	6.40906059286E-02	2.49042612428E+00	6.08507481241E-01
8.32744072957E-03	1.46429370558E+00	1.01811085298E+03	6.21143568124E-02	2.40200237414E+00	6.34960391986E-01
5.82920851070E-03	1.70150705501E+00	9.45885943182E+02	6.04607220009E-02	2.31871415076E+00	6.59118674130E-01
4.08044595749E-03	1.98624151552E+00	8.78179516689E+02	5.90717545333E-02	2.24771282885E+00	6.81258770140E-01
2.85631217024E-03	2.32917411173E+00	8.14482424576E+02	5.79010348087E-02	2.19737383638E+00	7.01639372893E-01
1.99941851917E-03	2.74346868897E+00	7.54363209114E+02	5.69111210919E-02	2.17731978186E+00	7.20498337609E-01
1.39959298342E-03	3.24536835562E+00	6.97445958483E+02	5.60716529140E-02	2.19841531059E+00	7.38044786219E-01

TABLE I (cont)

3.39022805648E-01	3.75258232023E-01	2.23824432615E+03	1.25801787855E-01	2.76703806377E+00	0.
3.89876295493E-01	3.57413796840E-01	2.30271579971E+03	1.32291776777E-01	2.73464559454E+00	0.
4.40357739817E-01	3.40108368706E-01	2.36885902504E+03	1.39530582383E-01	2.69626373469E+00	0.
5.15611400789E-01	3.23122206209E-01	2.43732625221E+03	1.47703292899E-01	2.65070713818E+00	0.
5.92953110908E-01	3.05921355398E-01	2.51022360011E+03	1.57226623621E-01	2.59513851470E+00	0.
6.81896077544E-01	2.85587923825E-01	2.60290384692E+03	1.70214693529E-01	2.51467004526E+00	0.
7.84180489175E-01	2.70075976505E-01	2.68440650788E+03	1.81507984082E-01	2.44026561179E+00	0.
9.01807562552E-01	2.57679360238E-01	2.75189522867E+03	1.91928120027E-01	2.37111998601E+00	0.

TABLE II

BKW EQUATION OF STATE FOR 1.7 g/cm^3 TATB

```
 A FORTRAN BKW CALCULATION FOR THE EXPLOSIVE
TATB     TRIAMINO  TRINITROBENZENE


THE NUMBER OF ELEMENTS IS      4


THE NUMBER OF GAS SPECIES IS    11


THE NUMBER OF SOLID SPECIES IS      1


THE BKW EQUATION OF STATE PARAMETERS ARE
 ALPHA= 5.00000000000E-01 BETA= 9.58500000000E-02 THETA= 4.00000000000E+02 KAPPA= 1.26847111054E+01


THE COMPOSITION OF THE EXPLOSIVE IS
     6.00000000000E+00 MOLES OF   C
     6.00000000000E+00 MOLES OF   H
     6.00000000000E+00 MOLES OF   N
     6.00000000000E+00 MOLES OF   O


THE DENSITY OF THE EXPLOSIVE IS  1.70000000000E+00, GRAMS/CC


THE MOLECULAR WEIGHT IS  2.58100000000E+02 GRAMS


THE HEAT OF FORMATION AT 0 DEG K IS -1.70000000000E+04 CALORIES PER FORMULA WEIGHT


THE SOLID (COWAN) EQUATION OF STATE PARAMETERS    VO, AS, BS, CS, DS, ES,     A1, A2, C1, C2, C3, ATOMIC WT


SOL C   4.44444444444E-01   8.30935837268E-01  -1.39381809219E+00   6.72569716021E-01  -1.13537262508E-01   6.49155882007E-
       -2.26705345948E-01,  1.20516569525E-01   8.31600000000E-02  -1.75590000000E-01   1.55310000000E-01   1.20100000000E+


THE INPUT DETONATION PRODUCT ELEMENTAL COMPOSITION MATRIX
 0.        2.0E+00  0.        1.0E+00  0.       2.0E+00  0.       0.       0.       0.       0.       2.0E+00
 1.0E+00   0.       0.        2.0E+00  1.0E+00  0.       0.       1.0E+00  0.       3.0E+00  1.0E+00  0.
 0.        1.0E+00  0.        0.       0.       0.       1.0E+00  1.0E+00  0.       0.       2.0E+00  0.
 0.        1.0E+00  0.        1.0E+00  1.0E+00  4.0E+00  0.       0.       1.0E+00  0.       0.       0.
```

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TABLE II (cont)

THE COMPUTED CJ PRESSURE IS 2.28936158051E-01 MEGABARS

THE COMPUTED DETONATION VELOCITY IS 7.24571592681E-01 CM/MICROSECOND

THE COMPUTED CJ TEMPERATURE IS 2.35061526358E+03 DEGREES KELVIN

THE COMPUTED CJ VOLUME 4.37348217576E-01 CC/GM OF EXPLOSIVE

THE COMPUTED GAMMA IS 2.89849639989E+00

THE VOLUME OF THE GAS IS 1.27224004502E+01 CC/MOLE OF GAS AND THERE ARE 7.51748535159E+00 MOLES OF GAS

SOLID	VOLUME IN CC/GM
SOL C	3.20240112536E-01

THE C-J COMPOSITION OF THE DETONATION PRODUCTS AND THE INPUT COEFFICIENTS TO THE THERMODYNAMIC FITS FOR EACH SPECIE

SPECIE	NO OF MOLES	COEFFICIENTS A,B,C,D,E, THE INTEGRATION	CONSTANT, HEAT OF	FORMATION IN CAL/MOLE,	COVOLUME	
H2O	2.99683858687E+00	4.25884200000E+01	1.48080500000E-02	-2.63913100000E-06	1.92045300000E-10	0.
		1.34282835156E+03	-5.71070000000E+04	2.50000000000E+02		
H2	2.76678289754E-03	2.97034700000E+01	1.14382900000E-02	-2.20122200000E-06	1.67776100000E-10	0.
		1.17589815365E+03	0.	8.00000000000E+01		
O2	1.58371087989E-07	4.70309000000E+01	1.28714700000E-02	-2.50021700000E-06	1.90157000000E-10	0.
		1.03537647396E+03	0.	3.50000000000E+02		
CO2	1.48540866079E+00	4.74811200000E+01	1.95446300000E-02	-3.72129600000E-06	2.77030000000E-10	0.
		7.46280968750E-02	-9.39680000000E+04	6.00000000000E+02		
CO	3.23298692254E-02	4.53308200000E+01	1.23816100000E-02	-2.41640300000E-06	1.82818100000E-10	0.
		1.12158830990E+03	-2.72010000000E+04	3.90000000000E+02		
NH3	2.49934496062E-04	4.20181600000E+01	1.91186200000E-02	-3.16433000000E-06	2.19780100000E-10	0.
		1.20698121615E+03	-9.36800000000E+03	4.76000000000E+02		
H	9.82201220537E-08	2.63911000000E+01	8.12137200000E-03	-1.69074000000E-06	1.31682300000E-10	0.
		7.94631617188E+02	5.16190000000E+04	4.00000000000E+01		
NO	1.41054926248E-05	4.84149800000E+01	1.26938600000E-02	-2.49460000000E-06	1.89321300000E-10	0.
		1.20924970573E+03	2.14770000000E+04	3.86000000000E+02		
N2	2.99986798001E+00	4.39234000000E+01	1.22250100000E-02	-2.37900500000E-06	1.79832200000E-10	0.
		1.13916134896E+03	0.	3.80000000000E+02		
OH	9.15733424094E-11	4.24179200000E+01	1.15684700000E-02	-2.22665900000E-06	1.68915500000E-10	0.
		1.18351754427E+03	3.56000000000E+03	4.13000000000E+02		
CH4	9.83966513327E-06	3.87568600000E+01	2.36401300000E-02	-3.70795700000E-06	2.47071400000E-10	0.
		1.04242791146E+03	-1.60000000000E+04	5.28000000000E+02		
SOL C	4.48225183032E+00	-2.46151900000E-01	7.17985500000E-03	-1.29755000000E-06	9.34999500000E-11	0.
		-2.58204389323E+02	0.	0.		

TABLE II (cont)

A BKW ISENTROPE THRU BKW CJ PRESSURE FOR
TATB TRIAMINO TRINITROBENZENE

LN(P)= -3.72405229051E+00 -2.59179870077E+00LNV 2.37983807393E-01LNV*2 7.68379923544E-02LNV*3 -2.82219705138E-02LNV*4

LN(T)= 7.32059840736E+00 -4.79994593935E-01LNV 7.48972735099E-02LNV*2 6.69368777648E-03LNV*3 -5.58045071334E-03LNV*4

LN(E)= -1.54467583100E+00 5.25610432064E-01LNP 9.29343272722E-02LNP*2 8.46907515126E-03LNP*3 3.10702193410E-04LNP*4

THE CONSTANT ADDED TO ENERGIES WAS 1.00000000000E-01

PRESSURE (MBARS)	VOLUME (CC/GM)	TEMPERATURE (DEG K)	ENERGY+C (MB-CC/GM)	GAMMA (-DLNP/DLNV)	PARTICLE VELOCITY
2.28838158051E-01	4.37348238625E-01	2.35061526358E+03	1.17271829353E-01	2.76391479619E+00	1.85858837839E-01
1.60255310636E-01	4.94602840279E-01	2.18643207959E+03	1.06288637944E-01	2.77324535879E+00	2.47241677227E-01
1.12178717445E-01	5.59814383498E-01	2.03525606358E+03	9.75337766553E-02	2.76830342293E+00	3.02656805521E-01
7.85251022114E-02	6.34919145171E-01	1.89604844811E+03	9.04777677462E-02	2.74986239609E+00	3.52996005178E-01
5.49675715480E-02	7.22347390566E-01	1.76892238567E+03	8.47567771138E-02	2.71833721708E+00	3.98933259310E-01
3.84773000836E-02	8.24748589080E-01	1.65061913106E+03	8.00340152753E-02	2.67414140409E+00	4.40833264864E-01
2.69341100585E-02	9.45742460083E-01	1.54203280105E+03	7.61276546180E-02	2.61761359957E+00	4.79125501010E-01
1.88538770410E-02	1.08871067878E+00	1.44251509954E+03	7.28739745424E-02	2.54927744243E+00	5.14122266751E-01
1.31977139287E-02	1.26217026199E+00	1.35140107379E+03	7.01462369293E-02	2.46990636785E+00	5.46107294150E-01
9.23839875007E-03	1.47012201414E+00	1.26797542583E+03	6.78450217163E-02	2.38061698550E+00	5.75348867012E-01
6.46687982505E-03	1.72304934005E+00	1.19236902591E+03	6.59090607360E-02	2.28276876821E+00	6.02155524808E-01
4.52681587753E-03	2.03148329106E+00	1.12207377472E+03	6.42415114544E-02	2.17884389449E+00	6.26675054844E-01
3.16877111427E-03	2.41038262103E+00	1.05707252348E+03	6.28077690790E-02	2.07149997420E+00	6.49188603366E-01
2.21813877988E-03	2.87855914916E+00	9.96612882138E+02	6.15678548175E-02	1.96430281865E+00	6.69927906418E-01
1.55268784588E-03	3.45884956630E+00	9.39231489310E+02	6.04771835052E-02	1.86190226770E+00	6.89075817390E-01
1.08888849220E-03	4.18593905700E+00	8.85913362311E+02	5.95384520343E-02	1.76912892591E+00	7.06949623373E-01
7.60821944537E-04	5.10015672073E+00	8.35206633817E+02	5.87088513355E-02	1.69264669738E+00	7.23713906783E-01
5.32575361176E-04	6.25617039096E+00	7.86615372537E+02	5.79784350515E-02	1.63990468507E+00	7.39575279391E-01
3.72802752823E-04	7.72572082231E+00	7.39735276790E+02	5.73248133144E-02	1.61987529128E+00	7.54726661463E-01
2.60961928878E-04	9.60265794581E+00	6.94246612514E+02	5.67418827798E-02	1.64225781471E+00	7.69336525724E-01
1.82673348883E-04	1.20088233107E+01	6.49888797040E+02	5.62182988880E-02	1.71816261805E+00	7.83528342324E-01
1.27871344218E-04	1.51012268827E+01	6.06493306232E+02	5.57472885568E-02	1.85941525022E+00	7.97348130003E-01
2.63278581758E-01	4.16714547039E-01	2.41870429518E+03	1.22335942122E-01	2.75609090468E+00	0.
3.02768088022E-01	3.98953772509E-01	2.48924220955E+03	1.27916621310E-01	2.74574490099E+00	0.
3.48183279375E-01	3.77984825746E-01	2.56227978477E+03	1.34084038720E-01	2.73270574175E+00	0.
4.00410771282E-01	3.59636217278E-01	2.63806884935E+03	1.40930445198E-01	2.71673450621E+00	0.
4.60472388874E-01	3.41822332467E-01	2.71706198424E+03	1.48583475008E-01	2.69746574043E+00	0.
5.29543245020E-01	3.24282424381E-01	2.80028557457E+03	1.57251038336E-01	2.67424676673E+00	0.
6.08874731773E-01	3.06414131852E-01	2.89095172364E+03	1.67412263324E-01	2.64546897293E+00	0.
7.00320941538E-01	2.85251130651E-01	3.00937809170E+03	1.81291048675E-01	2.60332292964E+00	0.
8.05369882770E-01	2.69250475440E-01	3.11480166055E+03	1.93253763162E-01	2.56444740260E+00	0.
9.26174445185E-01	2.56597539725E-01	3.20322090236E+03	2.04175816081E-01	2.52859989422E+00	0.

TABLE III

BKW EQUATION OF STATE FOR 1.8 g/cm^3 TATB

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 A FORTRAN BKW CALCULATION FOR THE EXPLOSIVE
TATB     TRIAMINO  TRINITROBENZENE


THE NUMBER OF ELEMENTS IS      4


THE NUMBER OF GAS SPECIES IS    11


THE NUMBER OF SOLID SPECIES IS     1


THE BKW EQUATION OF STATE PARAMETERS ARE
 ALPHA= 5.00000000000E-01 BETA= 9.58500000000E-02 THETA= 4.00000000000E+02 KAPPA= 1.26847111054E+01


THE COMPOSITION OF THE EXPLOSIVE IS
     6.00000000000E+00 MOLES OF   C
     6.00000000000E+00 MOLES OF   H
     6.00000000000E+00 MOLES OF   N
     6.00000000000E+00 MOLES OF   O


THE DENSITY OF THE EXPLOSIVE IS  1.80000000000E+00. GRAMS/CC


THE MOLECULAR WEIGHT IS  2.58100000000E+02 GRAMS


THE HEAT OF FORMATION AT 0 DEG K IS -1.70000000000E+04 CALORIES PER FORMULA WEIGHT


THE SOLID (COWAN) EQUATION OF STATE PARAMETERS    VO, AS, BS, CS, DS, ES,     A1, A2, C1, C2, C3, ATOMIC WT


SOL C   4.44444444444E-01   8.30935837268E-01  -1.39381809219E+00   6.72569716021E-01  -1.13537262508E-01   6.49155882007E-
       -2.26705345948E-01   1.20516569525E-01   8.31600000000E-02  -1.75590000000E-01   1.55310000000E-01   1.20100000000E+


THE INPUT DETONATION PRODUCT ELEMENTAL COMPOSITION MATRIX
  0.        2.0E+00   0.        1.0E+00   0.        2.0E+00   0.        0.        0.        0.        0.        2.0E+00
  1.0E+00   0.        0.        2.0E+00   1.0E+00   0.        0.        1.0E+00   0.        3.0E+00   1.0E+00   0.
  0.        1.0E+00   0.        0.        0.        0.        1.0E+00   1.0E+00   0.        0.        2.0E+00   0.
  0.        1.0E+00   0.        1.0E+00   1.0E+00   4.0E+00   0.        0.        1.0E+00   0.        0.        0.
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TABLE III (cont)

THE COMPUTED CJ PRESSURE IS 2.62334113015E-01 MEGABARS

THE COMPUTED DETONATION VELOCITY IS 7.55551363678E-01 CM/MICROSECOND

THE COMPUTED CJ TEMPERATURE IS 2.23925687971E+03 DEGREES KELVIN

THE COMPUTED CJ VOLUME 4.13721632585E-01 CC/GM OF EXPLOSIVE

THE COMPUTED GAMMA IS 2.91692922384E+00

THE VOLUME OF THE GAS IS 1.20051822376E+01 CC/MOLE OF GAS AND THERE ARE 7.50765517275E+00 MOLES OF GAS

SOLID	VOLUME IN CC/GM
SOL C	3.08622308022E-01

THE C-J COMPOSITION OF THE DETONATION PRODUCTS AND THE INPUT COEFFICIENTS TO THE THERMODYNAMIC FITS FOR EACH SPECIE

SPECIE	NO OF MOLES	COEFFICIENTS A,B,C,D,E, THE INTEGRATION CONSTANT, HEAT OF FORMATION IN CAL/MOLE,COVOLUME				
H2O	2.99881673313E+00	4.25884200000E+01	1.48080500000E-02	-2.63918100000E-06	1.92045300000E-10	0.
		1.34282835156E+03	-5.71070000000E+04	2.50000000000E+02		
H2	1.04451656564E-03	2.97034700000E+01	1.14382900000E-02	-2.20122200000E-06	1.67776100000E-10	0.
		1.17589615365E+03	0.	8.00000000000E+01		
O2	8.84284327135E-08	4.70309000000E+01	1.28714700000E-02	-2.50021700000E-06	1.90157000000E-10	0.
		1.03537647398E+03	0.	3.50000000000E+02		
CO2	1.49343248805E+00	4.74811200000E+01	1.95446300000E-02	-3.72129600000E-06	2.77030000000E-10	0.
		7.46280968750E+02	-9.39680000000E+04	6.00000000000E+02		
CO	1.43106371873E-02	4.53308200000E+01	1.23816100000E-02	-2.41640300000E-06	1.82818100000E-10	0.
		1.12158830990E+03	-2.72010000000E+04	3.90000000000E+02		
NH3	8.98005989069E-05	4.20181600000E+01	1.91166200000E-02	-3.16433000000E-06	2.19780100000E-10	0.
		1.20696121615E+03	-9.36800000000E+03	4.76000000000E+02		
H	5.44860972415E-10	2.63911000000E+01	8.12137200000E-03	-1.69074000000E-06	1.31682300000E-10	0.
		7.94631817188E+02	5.16190000000E+04	4.00000000000E+01		
NO	7.47633553468E-06	4.84149800000E+01	1.26938600000E-02	-2.49460000000E-06	1.89321300000E-10	0.
		1.20924970573E+03	2.14770000000E+04	3.86000000000E+02		
N2	2.99995135753E+00	4.39234000000E+01	1.22250100000E-02	-2.37900500000E-06	1.79832200000E-10	0.
		1.13916134896E+03	0.	3.80000000000E+02		
OH	3.85580145325E-10	4.24179200000E+01	1.15684700000E-02	-2.22665900000E-06	1.68915500000E-10	0.
		1.18351754427E+03	3.56000000000E+03	4.13000000000E+02		
CH4	2.01847197399E-06	3.87568600000E+01	2.36401300000E-02	-3.70795700000E-06	2.47071400000E-10	0.
		1.04242791146E+03	-1.60000000000E+04	5.28000000000E+02		
SOL C	4.49225485629E+00	-2.46151900000E-01	7.17985500000E-03	-1.29755000000E-06	9.34999500000E-11	0.
		-2.58204389323E+02	0.	0.		

TABLE III (cont)

A BKW ISENTROPE THRU BKW CJ PRESSURE FOR
TATB TRIAMINO TRINITROBENZENE

LN(P)= -3.77999581511E+00 -2.64275097989E+00LNV 2.37019602784E-01LNV+2 8.26760800509E-02LNV+3 -3.05845127183E-02LNV+4

LN(T)= 7.23117772892E+00 -5.00269717709E-01LNV 6.49199742507E-02LNV+2 8.23572478691E-03LNV+3 -6.18626956109E-03LNV+4

LN(E)= -1.56612716340E+00 5.36464548171E-01LNP 9.60475159250E-02LNP+2 8.75007889874E-03LNP+3 3.18881552649E-04LNP+4

THE CONSTANT ADDED TO ENERGIES WAS 1.00000000000E-01

PRESSURE (MBARS)	VOLUME (CC/GM)	TEMPERATURE (DEG K)	ENERGY+C (MB-CC/GM)	GAMMA (-DLNP/DLNV)	PARTICLE VELOCITY
2.62334113015E-01	4.13721632022E-01	2.23925687971E+03	1.18604008912E-01	2.78382666451E+00	1.92893432698E-01
1.83633879111E-01	4.67270067662E-01	2.08326224720E+03	1.06830195741E-01	2.80595835216E+00	2.56407444926E-01
1.28543715378E-01	5.27759538979E-01	1.93883156137E+03	9.75224827148E-02	2.81246761957E+00	3.13470294135E-01
8.99806007643E-02	5.96896159020E-01	1.80528161225E+03	9.00780093542E-02	2.80450986945E+00	3.65113677837E-01
6.29864205350E-02	6.76708226114E-01	1.68192648660E+03	8.40638855771E-02	2.78275986647E+00	4.12056218534E-01
4.40904943745E-02	7.69761019177E-01	1.56906191759E+03	7.91809871451E-02	2.74761976910E+00	4.54869397880E-01
3.08633460622E-02	8.78845560218E-01	1.46380958098E+03	7.51471355274E-02	2.69957098556E+00	4.93863494742E-01
2.16043422435E-02	1.00778108810E+00	1.36691350862E+03	7.18101170564E-02	2.63906187153E+00	5.29429966825E-01
1.51230385705E-02	1.16118263085E+00	1.27771125741E+03	6.90315896525E-02	2.56678034296E+00	5.61862374673E-01
1.05861276993E-02	1.34483711202E+00	1.19551240624E+03	6.67040421688E-02	2.48371621835E+00	5.91432626710E-01
7.41028938952E-03	1.56603377851E+00	1.11959788394E+03	6.47429611554E-02	2.39126115486E+00	6.18399015293E-01
5.18720257267E-03	1.83397224395E+00	1.04924772414E+03	6.30814584995E-02	2.29131419031E+00	6.43008803543E-01
3.63104180087E-03	2.16027350096E+00	9.83770018445E+02	6.16662788324E-02	2.18638628896E+00	6.65499197664E-01
2.54172926061E-03	2.55965008486E+00	9.22522709026E+02	6.04547404696E-02	2.07968814078E+00	6.86099059001E-01
1.77921048242E-03	3.05081303738E+00	8.64925024795E+02	5.94123635846E-02	1.97519390266E+00	7.05030922931E-01
1.24544733770E-03	3.65769898953E+00	8.10462011686E+02	5.85110887386E-02	1.87768990128E+00	7.22511913005E-01
8.71813136388E-04	4.41108898934E+00	7.58683807699E+02	5.77279758718E-02	1.79282509515E+00	7.38752741220E-01
6.10269195472E-04	5.35067252223E+00	7.09200414176E+02	5.70442641651E-02	1.72716937258E+00	7.53954926388E-01
4.27188438830E-04	6.52757571039E+00	6.61672986610E+02	5.64446722831E-02	1.68826332455E+00	7.68306211363E-01
2.99031905781E-04	8.00730115144E+00	6.15804462186E+02	5.59168507194E-02	1.68461848649E+00	7.81973064965E-01
2.09322334047E-04	9.87288543842E+00	5.71332360225E+02	5.54509318346E-02	1.72560723927E+00	7.95088003519E-01
1.46525633833E-04	1.22278225843E+01	5.28024600477E+02	5.50391510230E-02	1.82117053980E+00	8.07729645604E-01
1.02567943683E-04	1.51978430966E+01	4.85676179181E+02	5.46755263268E-02	1.98127002193E+00	8.19896499795E-01
3.01684229988E-01	3.94295071884E-01	2.30365042342E+03	1.24067809319E-01	2.77048427655E+00	0.
3.48838884463E-01	3.75605315680E-01	2.37019488969E+03	1.30116438625E-01	2.75424480137E+00	0.
3.98877384132E-01	3.57540112911E-01	2.43895474946E+03	1.36840382448E-01	2.73483082259E+00	0.
4.58824003252E-01	3.39952221161E-01	2.51029269470E+03	1.44369473120E-01	2.71181594165E+00	0.
5.27647603740E-01	3.22589145147E-01	2.58509996799E+03	1.52919296885E-01	2.68442181370E+00	0.
6.06794744301E-01	3.04779481884E-01	2.66644130089E+03	1.63012354920E-01	2.65062940130E+00	0.
6.97813955946E-01	2.83344130491E-01	2.77391244805E+03	1.77011367482E-01	2.60074581891E+00	0.
8.02486049338E-01	2.68110048602E-01	2.86315306446E+03	1.88369169615E-01	2.55792253128E+00	0.
9.22858956739E-01	2.55712688481E-01	2.93928735384E+03	1.99033077480E-01	2.51769048143E+00	0.

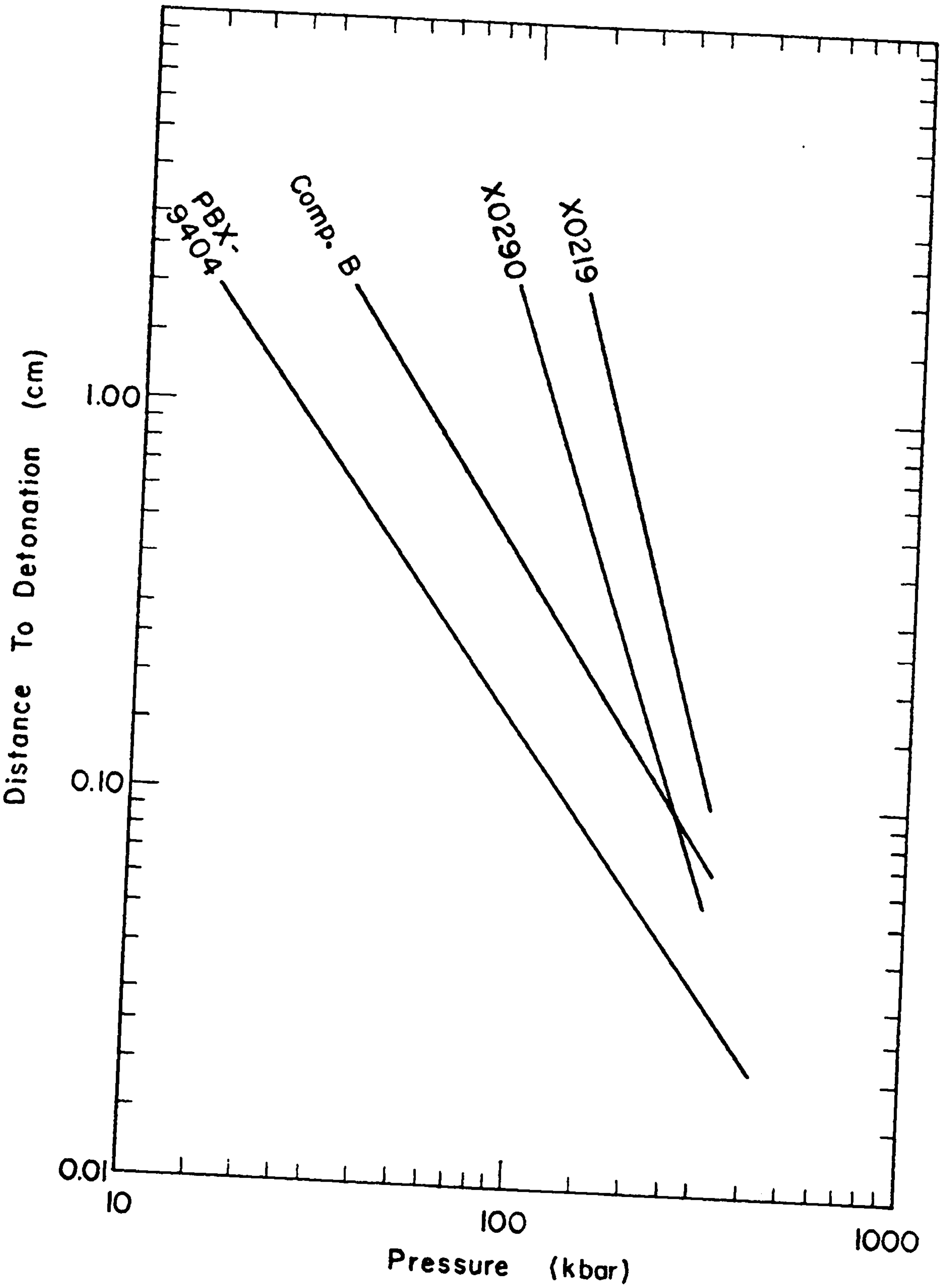

Fig. 1.
The distance of run to detonation as a function of the shock pressure.

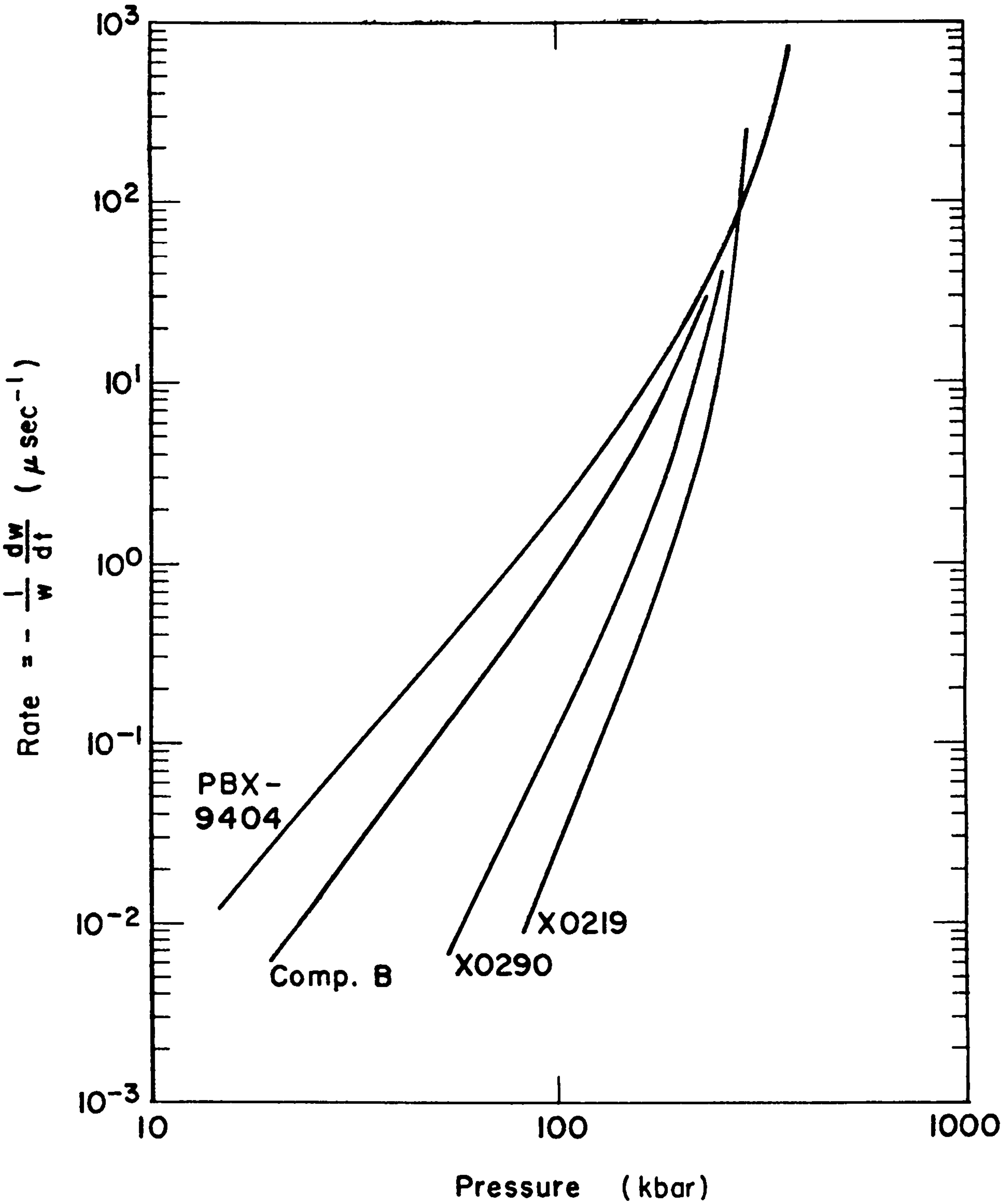

Fig. 2
The Forest Fire decomposition rates as a function of shock pressure.

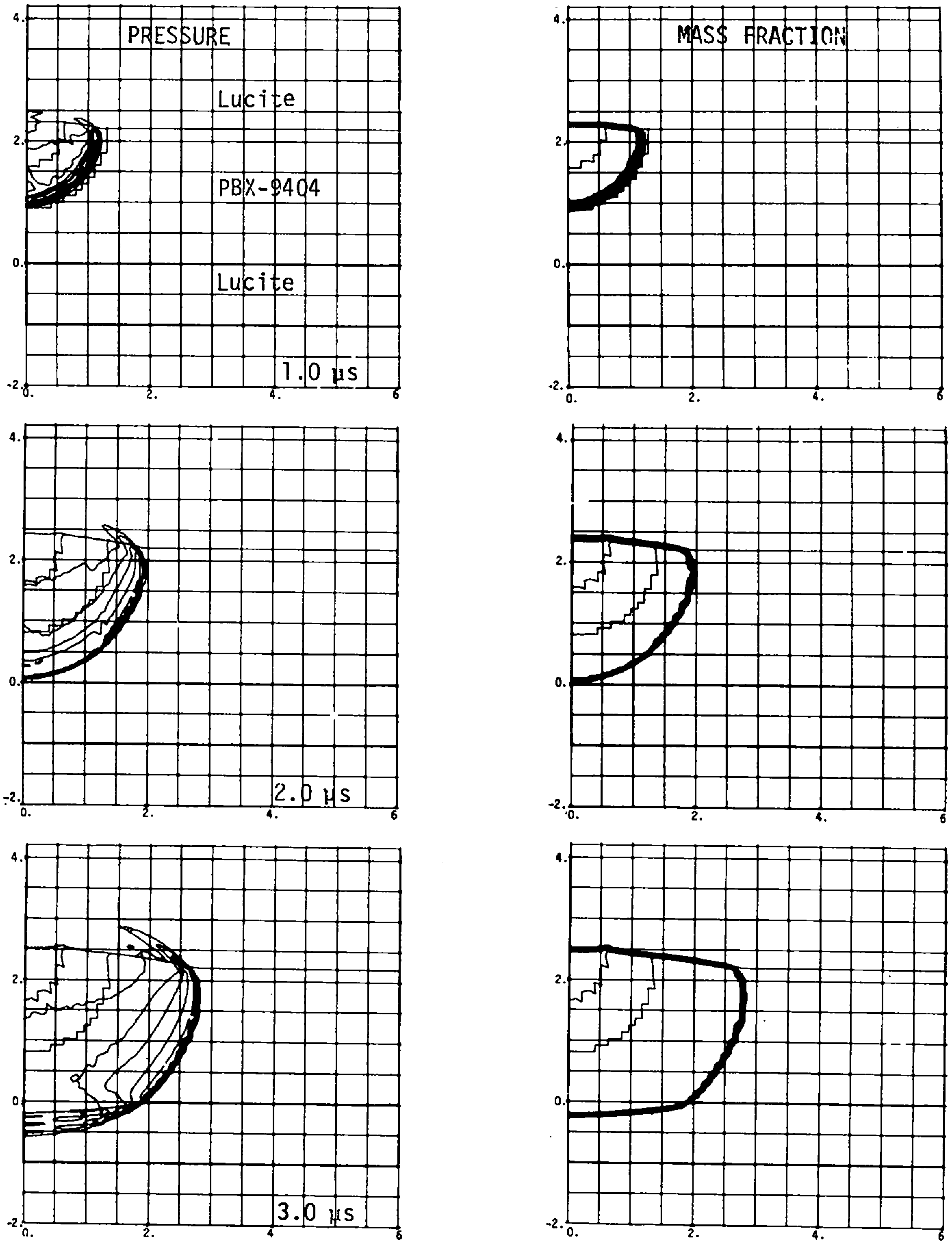

Fig. 3.
The pressure and mass fraction contours at various times for a hemispherical initiator of 6.35-mm-radius PBX-9407 surrounded by 6.35 mm of PBX-9404 initiating PBX-9404. The pressure contour interval is 50 kbar and the mass fraction contour is 0.1.

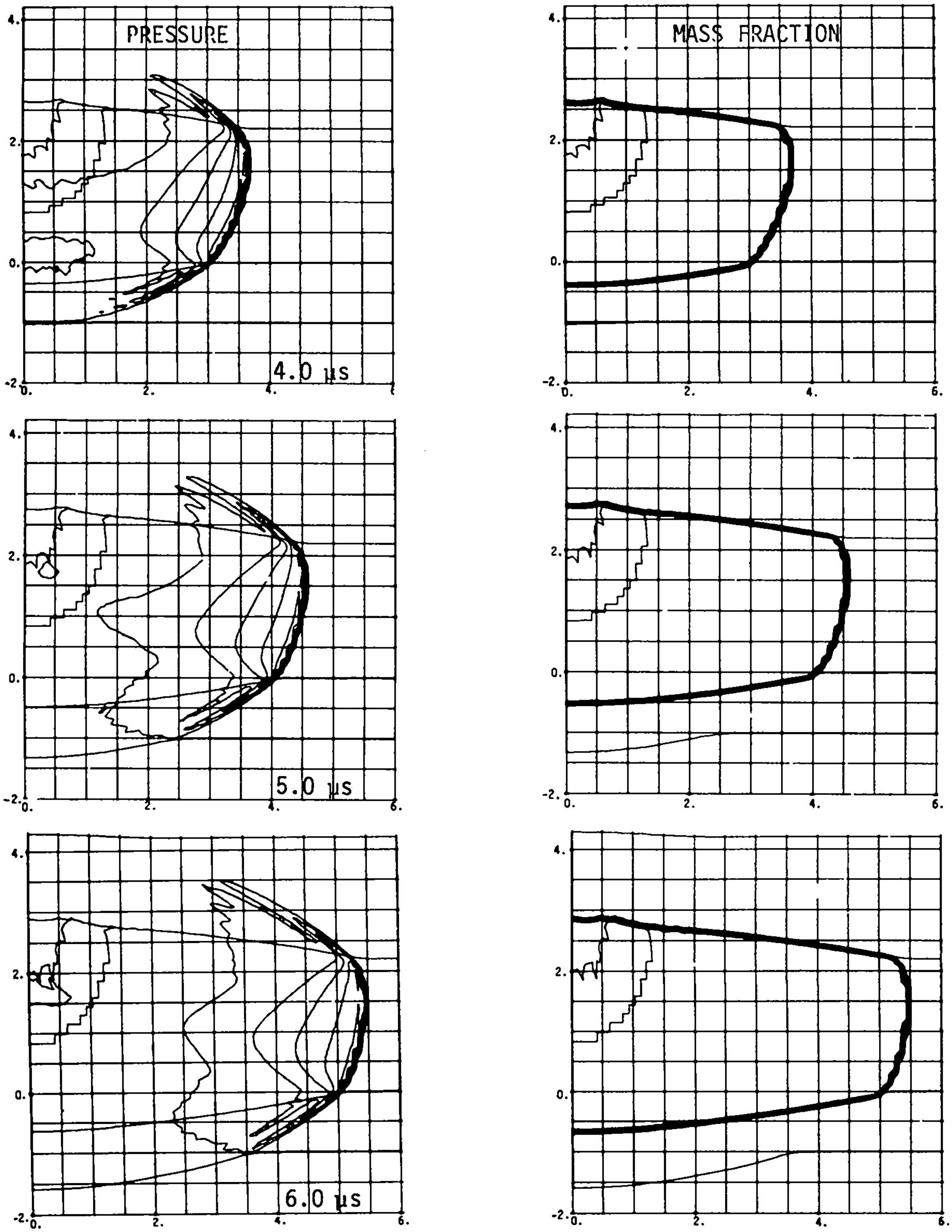

Fig. 3. (cont)

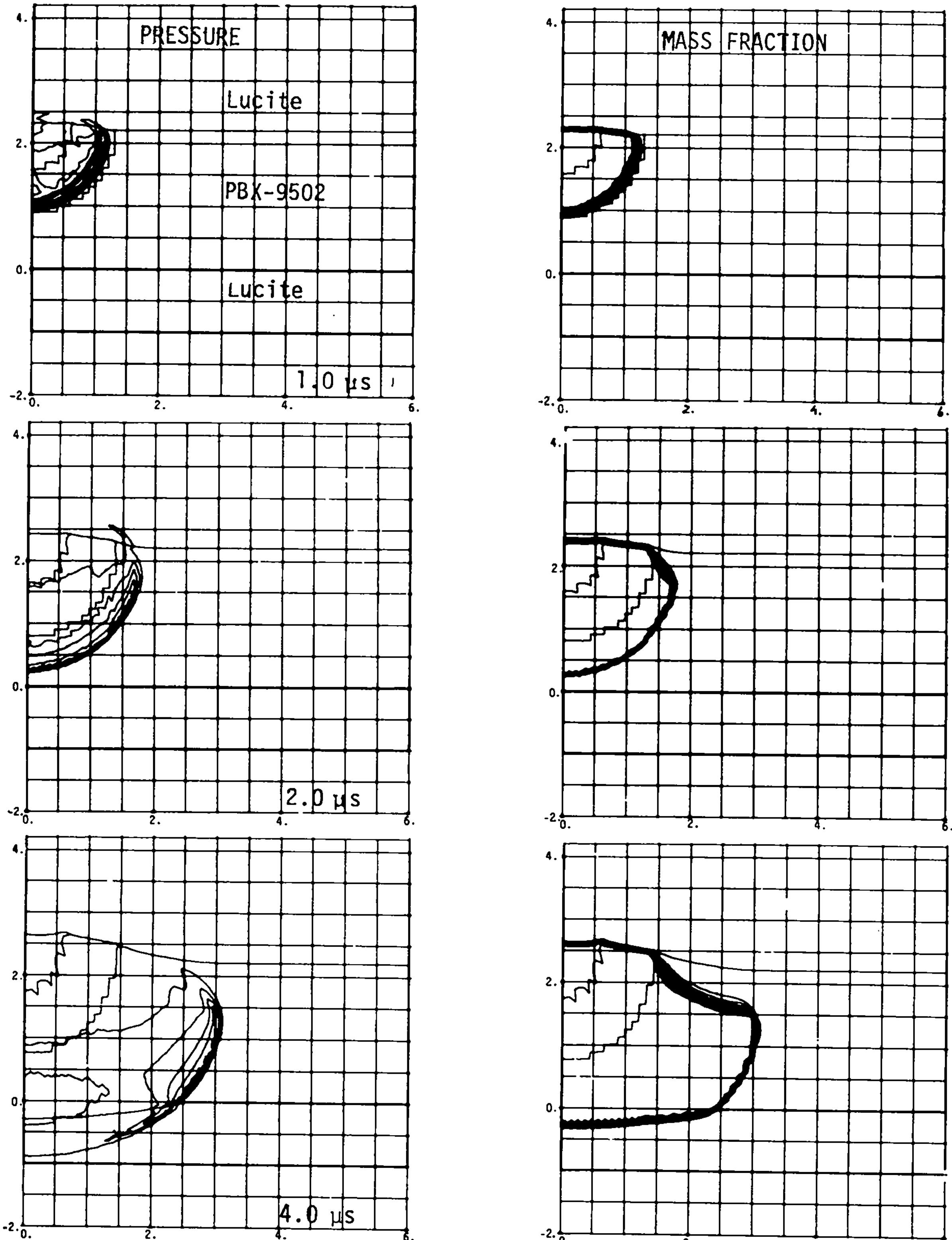

Fig. 4.

The pressure and mass fraction contours at various times for a hemispherical initiator of 6.35-mm-radius PBX-9407 surrounded by 6.35 mm of PBX-9404 initiating PBX-9502 (X0290). The pressure contour interval is 50 kbar and the mass fraction contour is 0.1.

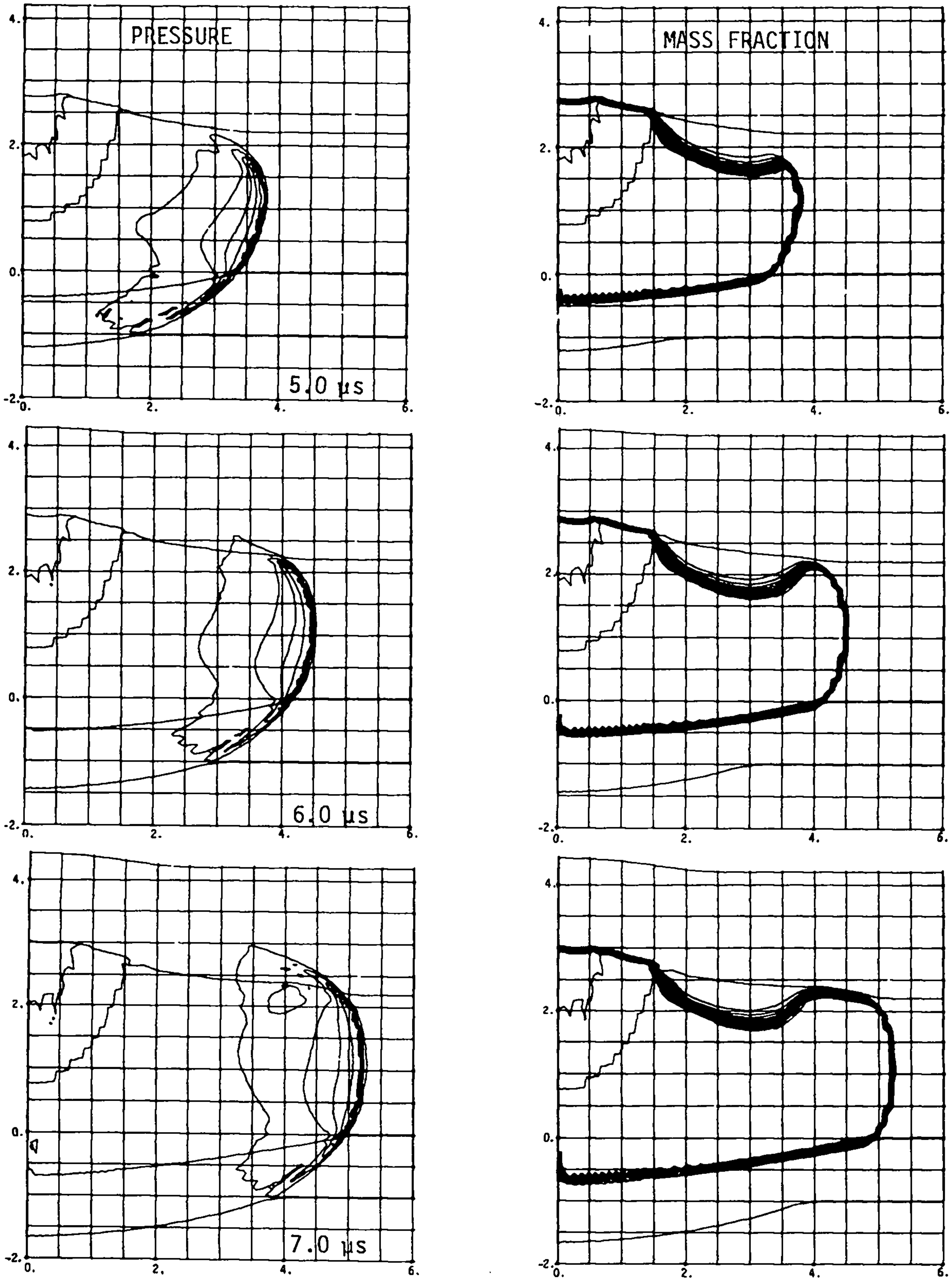

Fig. 4. (cont)

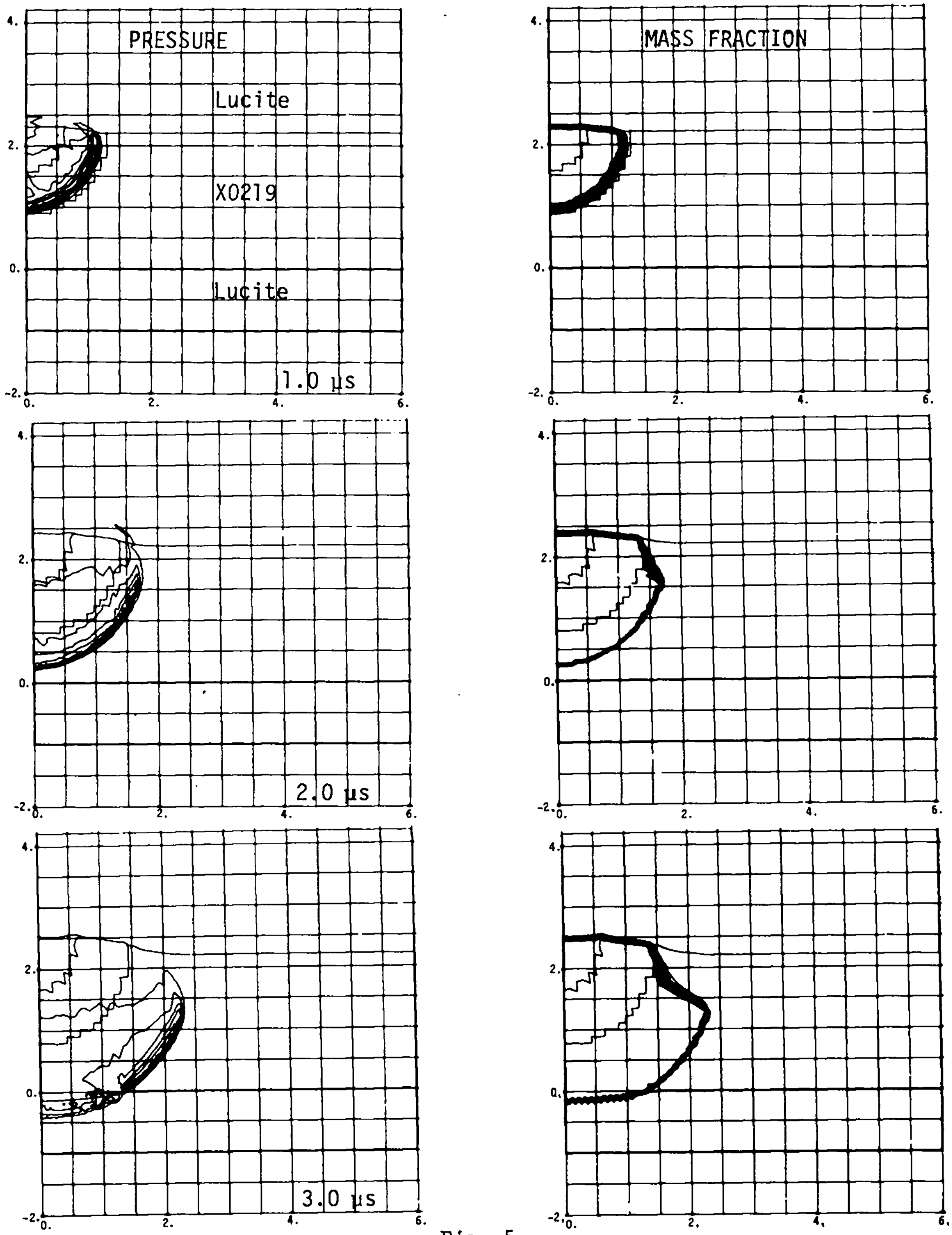

Fig. 5.
The pressure and mass fraction contours at various times for a hemispherical initiator of 6.35-mm-radius PBX-9407 surrounded by 6.35 mm of PBX-9404 initiating X0219. The pressure contour interval is 50 kbar and the mass fraction contour is 0.1.

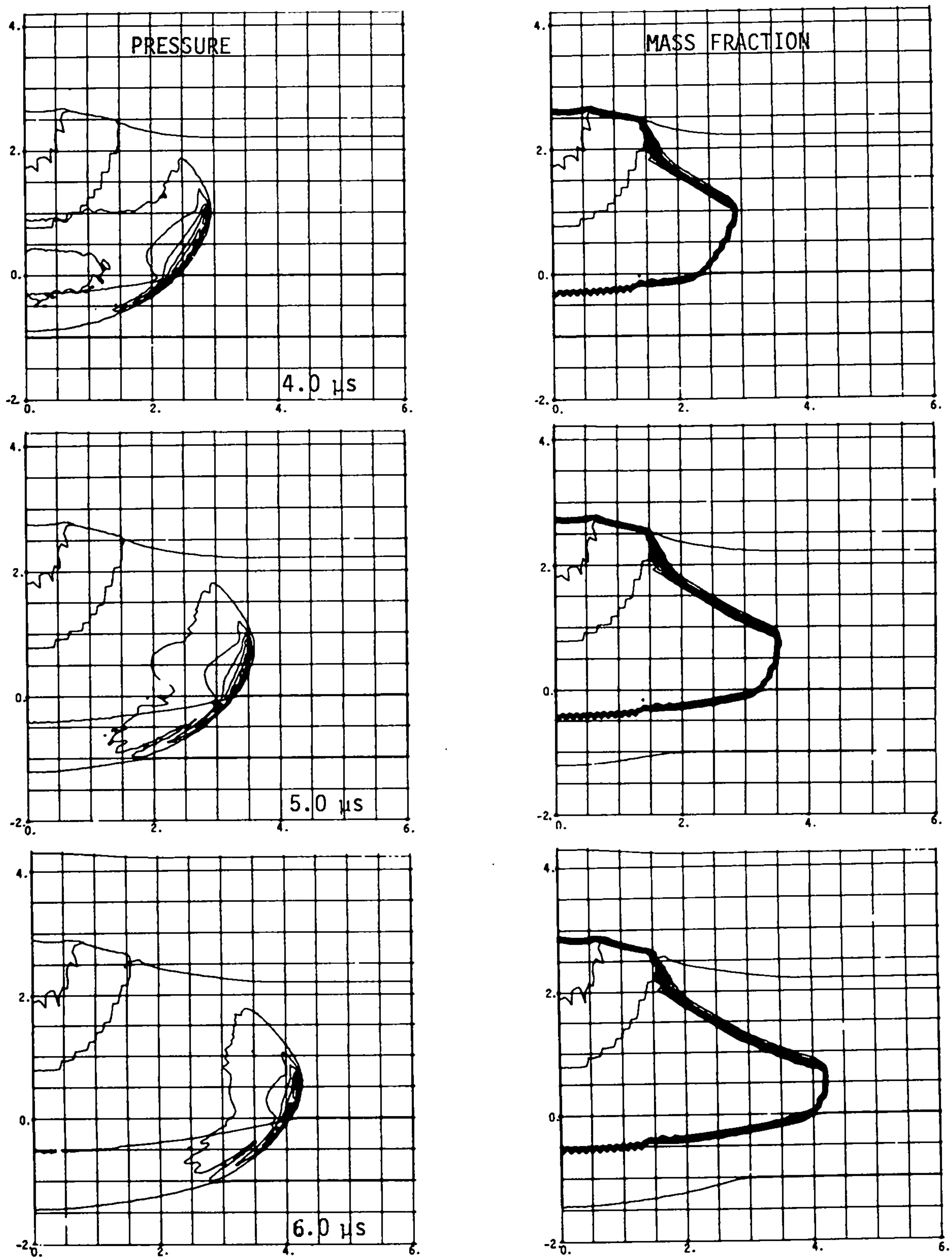

Fig. 5. (cont)

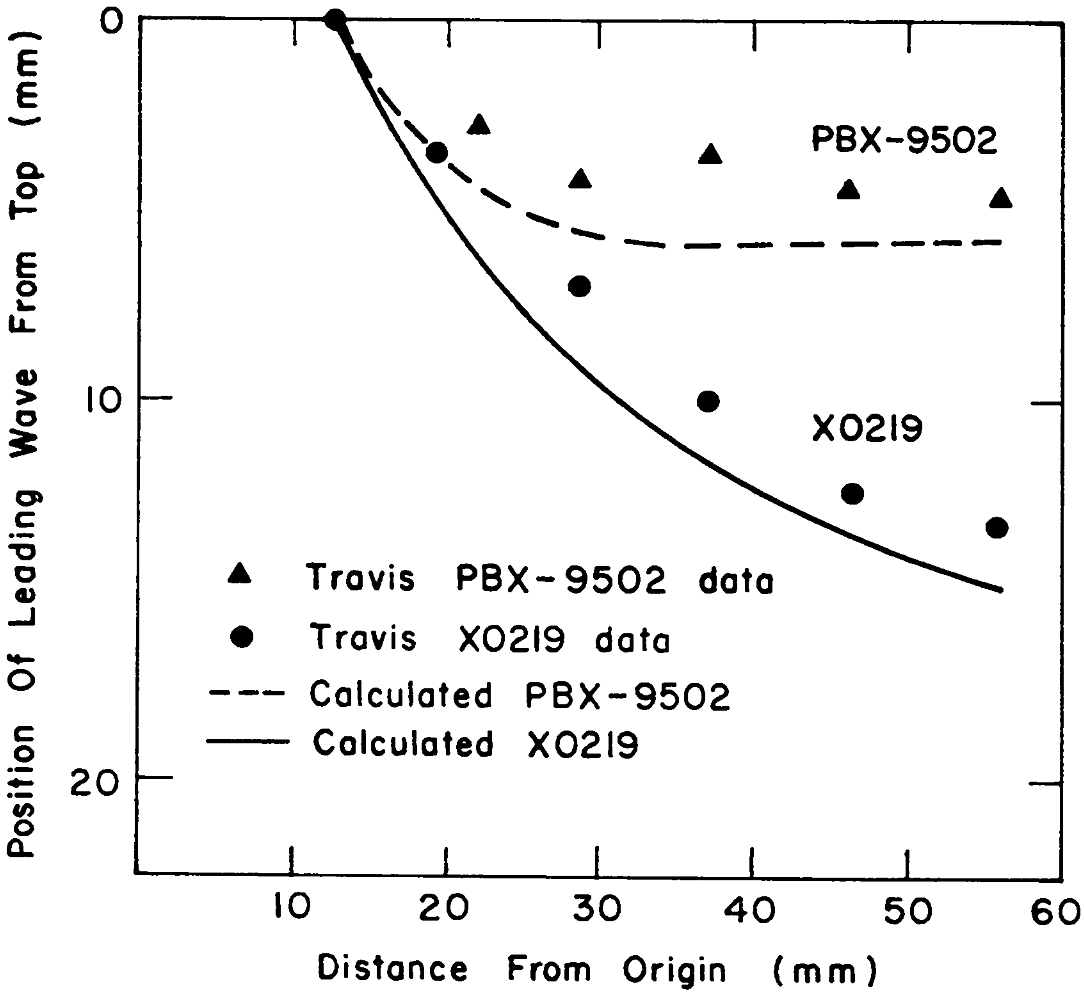

Fig. 6.
The experimental and calculated position of the leading wave from the top of the explosive block as a function of the distance of the leading front of the wave from the origin.

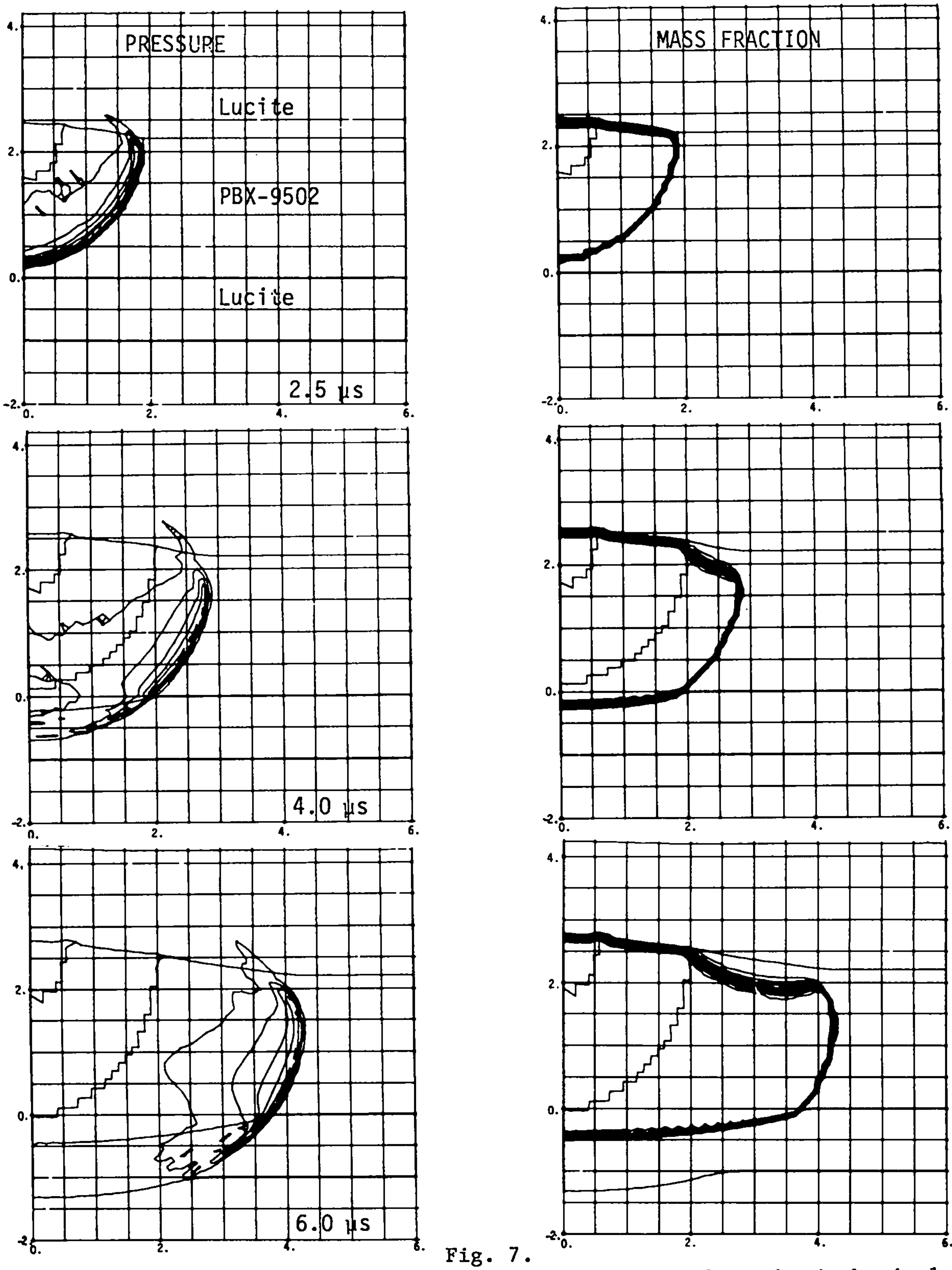

Fig. 7.
The pressure and mass fraction contours at various times for a hemispherical initiator of 6.35-mm-radius TATB at 1.7 g/cm^3 surrounded by 19.05 mm of TATB at 1.8 g/cm^3 initiating PBX-9502. The pressure contour interval is 50 kbar and the mass fraction contour is 0.1.

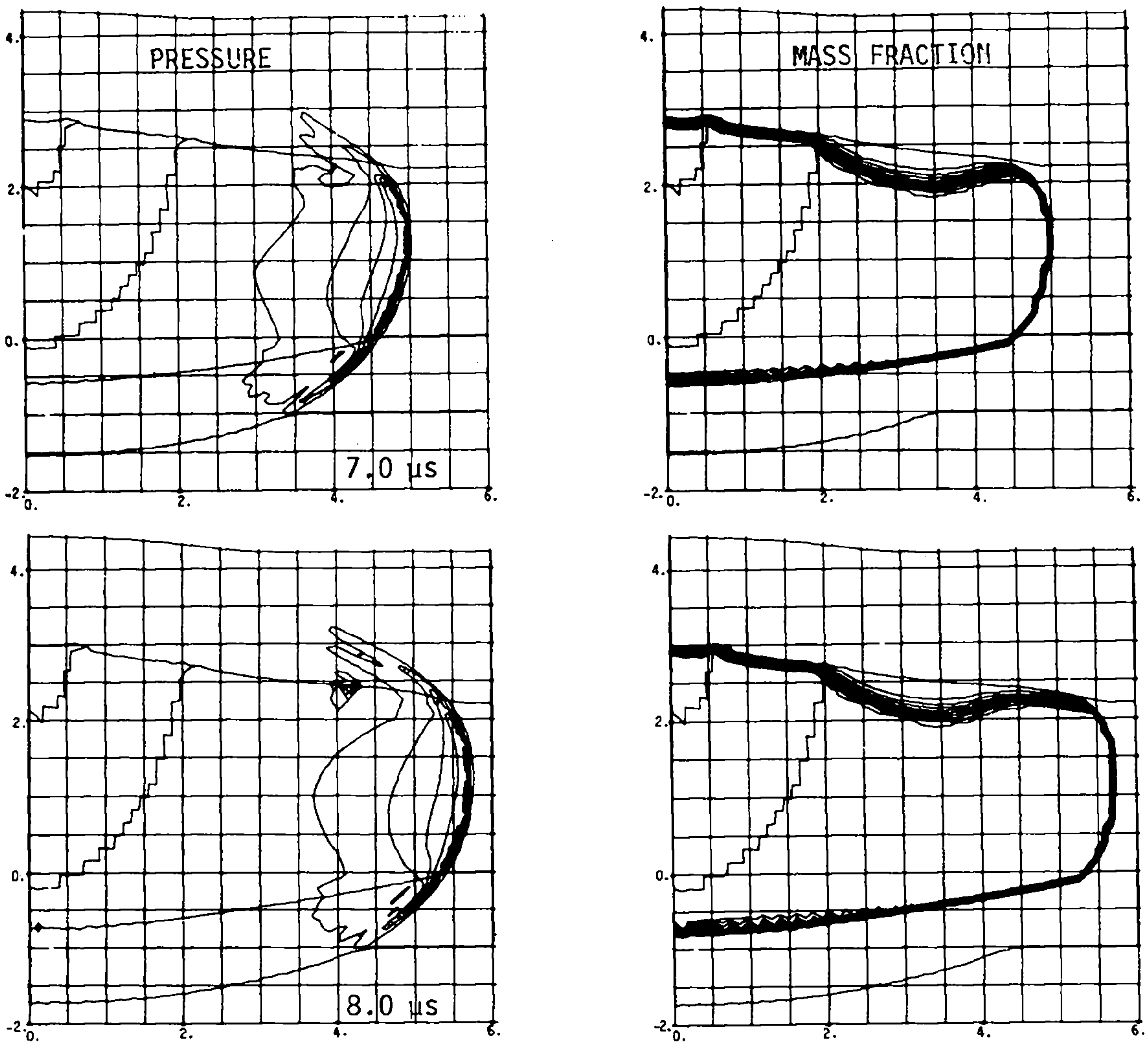

Fig. 7. (cont)

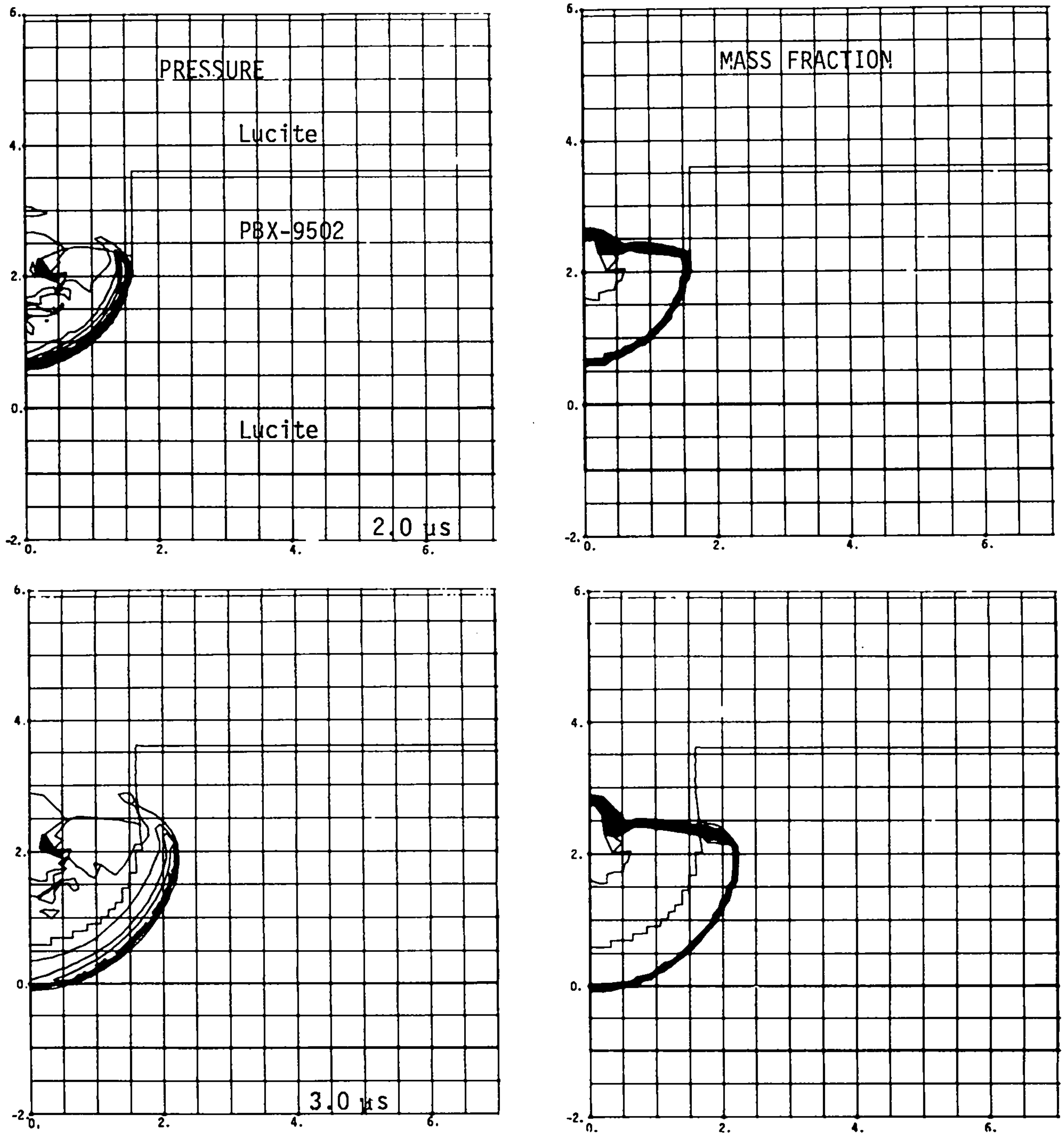

Fig. 8.
The pressure and mass fraction contours at various times for a hemispherical initiator of 16-mm-radius X0351 initiating PBX-9502. The pressure contour interval is 50 kbar and the mass fraction contour is 0.1.

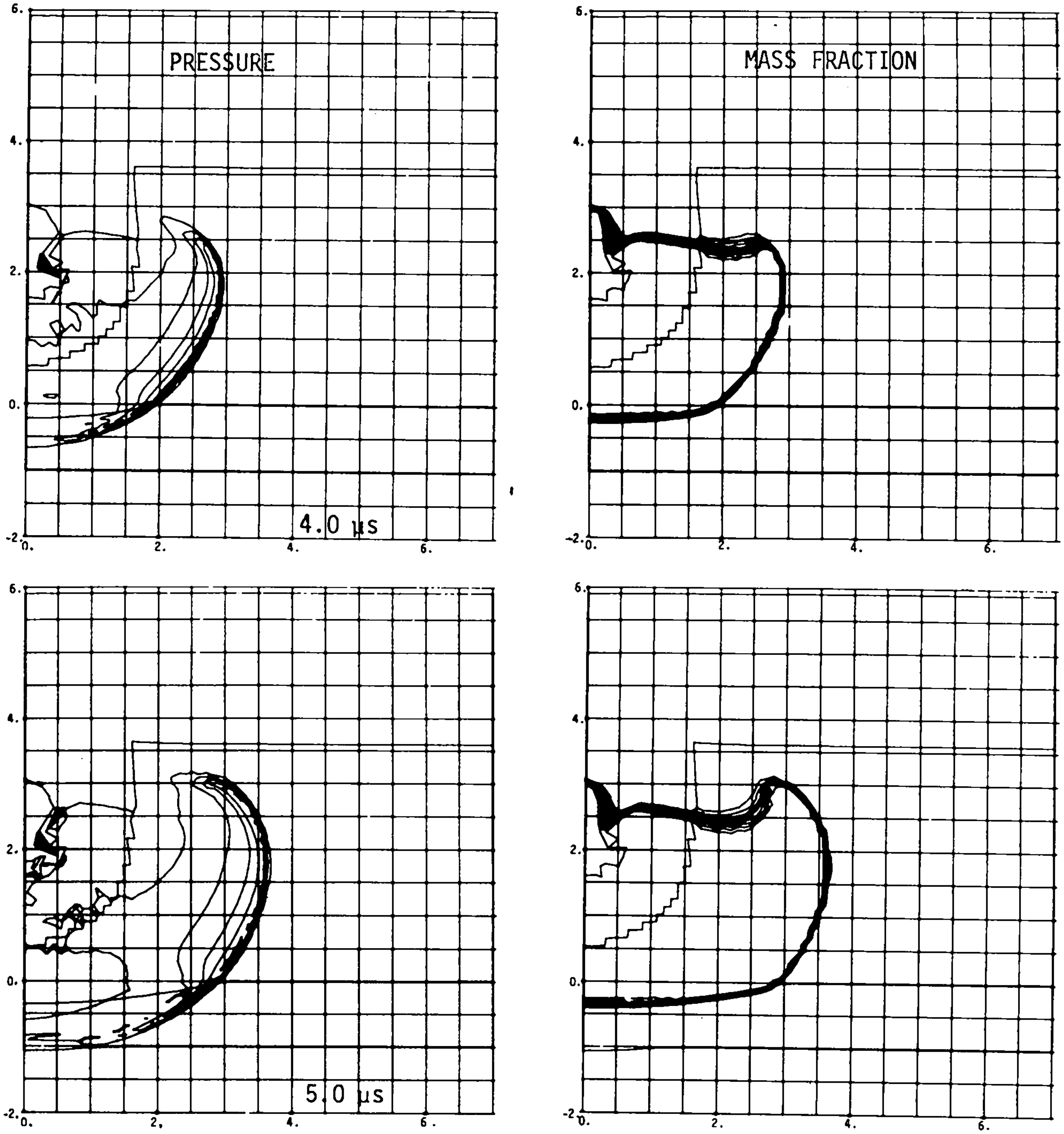

Fig. 8. (cont)

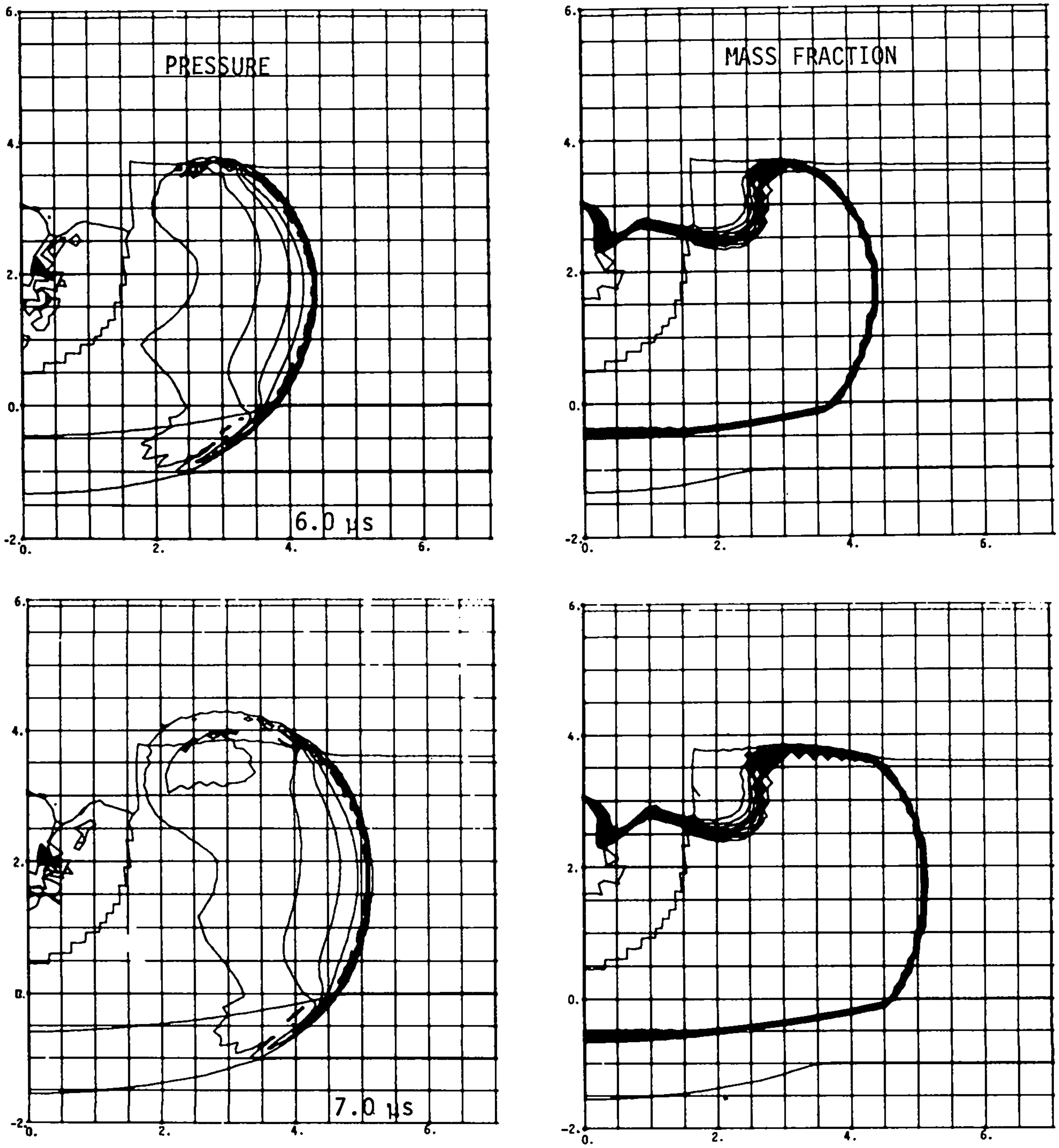

Fig. 8. (cont)

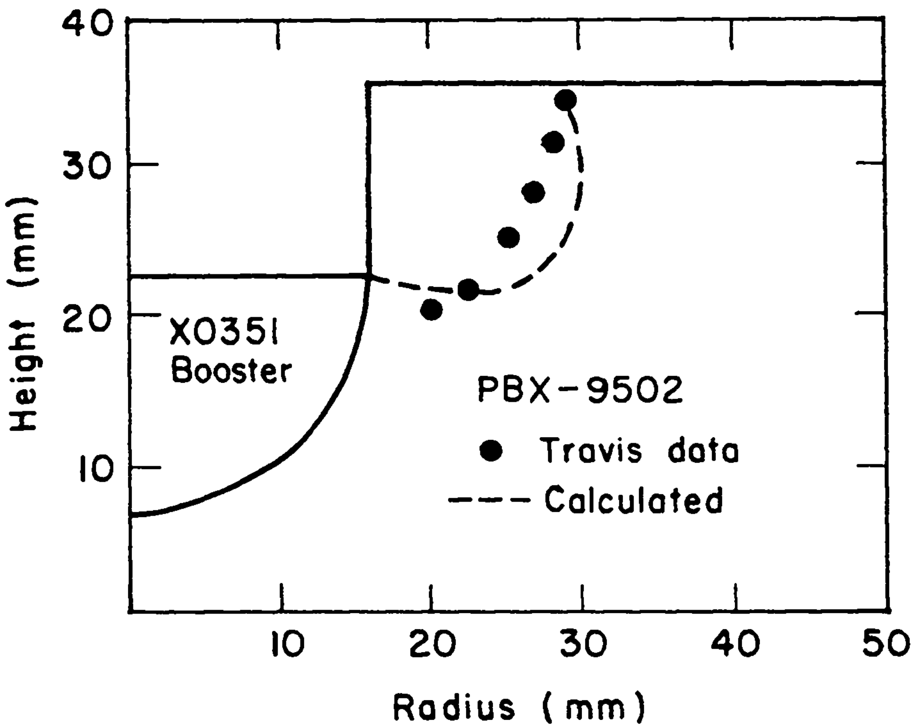

Fig. 9.
The calculated and experimental region of partially decomposed PBX-9502 when initiated by an X0351 initiator.

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