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Consistency among Differential Nuclear Data and Integral Observations: The ALVIN Code for Data Adjustment, for Sensitivity Calculations, and for Identification of Inconsistent Data

by

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CONTENTS

		. т
I.	INTRODUCTION	. 1
II.	CONSISTENCY TESTS AND DATA ADJUSTMENT	. 2
	A. Tests for Consistency Among Differential and Integral Data	. 3
	B. Nuclear Data Adjustment	. 4
	1. Data Adjustment with Full Correlations - DAFT2	. 5
	2. Adjustment of Arbitrarily Large Differential Data Sets - DAFT3	. 6
III.	SENSITIVITY CALCULATIONS	. 7
	A. Inhomogeneous Transport	. 7
•	B. Reactivity, Rossi- α , and Other Eigenproblems	. 9
	C. Sensitivity Profile	. 11
IV.	ALVIN PROGRAMMING	. 12
v.	SAMPLE PROBLEMS AND CODE VALIDATION	. 13
	A. Data Consistency and Adjustment	. 13
	B. Sensitivity Calculation	. 16
VI.	INPUT AND OUTPUT	. 17
VII.	SUMMARY OF ALVIN CAPABILITIES AND LIMITATIONS	. 17
	ACKNOWLEDGMENTS	. 18
	REFERENCES	. 18
APPENDIX A.	PROGRAM ABSTRACT	. 20
APPENDIX B.	DEFINITIONS OF VARIABLES USED IN ALVIN	. 21
APPENDIX C.	SAMPLE INPUT FOR DATA CONSISTENCY AND ADJUSTMENT PROBLEM	. 23
APPENDIX D.	SAMPLE OUTPUT FOR DATA CONSISTENCY AND ADJUSTMENT PROBLEM	. 25
APPENDIX E.	SAMPLE INPUT FOR SENSITIVITY CALCULATION	31
APPENDIX F.	SAMPLE OUTPUT FOR SENSITIVITY CALCULATION	. 31
	TABLES	
25 · · · ·	ROUTINE CALLS AND TAPE REQUIREMENTS IN ALVIN	12
4 tr.	INTEGRAL PARAMETERS y, AND VALUES y ₁ (x ^e) COMPUTED USING EVALUATED NUCLEAR DATA PARAMETERS x _e	. 14
0037	PRIMARY NUCLEAR DATA PARAMETERS x, THEIR UNCERTAINTIES, AND THEIR ADJUSTED VALUES	. 14
1v.	SENSITIVITY COEFFICIENTS (xj/yi) 3yi/3xj FOR ZPR-6-6A, ZPR-6-7, AND ZPR-3-48	15
v.	ALVIN PROBLEM INPUT	18

FIGURES

1.	ALVIN Structure	13
2.	Sensitivity of shield surface neutron dose-equivalent rate to neutron cross-section data computed by direct change in cross sections and by linear perturbation ALVIN calculation	17

CONSISTENCY AMONG DIFFERENTIAL NUCLEAR DATA

AND INTEGRAL OBSERVATIONS: THE ALVIN CODE FOR DATA ADJUSTMENT,

FOR SENSITIVITY CALCULATIONS, AND FOR IDENTIFICATION OF INCONSISTENT DATA

bу

D. R. Harris, W. A. Reupke, and W. B. Wilson

ABSTRACT

Successful nuclear design requires adequate prediction of integral design parameters, and this in turn requires an adequate differential nuclear data base. Data bases that apparently permit reduced biases and design margins have been developed by a) least squares adjustment of differential data or b) trial-and-error selection from alternative evaluated data sets. Criticisms and defenses of such procedures are discussed. We relate useful data adjustment to consistency of the combined differential-integral data set, and we describe consistency tests related to least squares adjustment procedures. We suggest an approach to data adjustment that is contingent on consistency analysis. A FORTRAN code ALVIN has been developed to carry out the indicated data consistency and adjustment calculations, and to compute required sensitivities of integral parameters to nuclear data changes. The sensitivity modules of ALVIN are validated by computing with two distinct methods the cross-section sensitivity profile for neutron penetration through a thick iron shield. The data consistency and adjustment modules DAFT2 (for arbitrary variance-covariance data) and DAFT3 (for differential data base of arbitrary size uncorrelated with integral data) are validated by comparing their results for a set of data for three ZPR criticals.

INTRODUCTION

Successful nuclear design requires adequate prediction of a number of integral design parameters. Among these are reactivity worths, energy deposition rates, nuclide transmutation rates, radiation doses, and Rossi-\alpha. Adequate prediction of integral design quantities requires, in turn, a recognizably adequate nuclear data base. Massive programs for measurement and analysis of differential and integral nuclear data have been devoted to this objective, and the end is not yet in sight.

In the meantime, "improved" nuclear data bases have been achieved, apparently permitting reduced design biases and margins, through a) data adjustment by least squares techniques, or b) trial-and-error selection among alternative data sets. Data adjustment or selection is carried out so as to improve agreement between calculations and measurements made on as-built nuclear devices and on special experiments devised to resemble them. Many

workers have contributed to this development. 1-26
It is generally supposed that the data adjustment or selection is not simply compensating for the systematic errors in computational technique; instead, errors in calculation are assumed to be driven down or allowed for as a result of numerical experimentation or as a result of comparison with very accurate methods such as continuous energy Monte Carlo.

Critics of data adjustment and selection strategies emphasize that forced but unphysical changes in data may yield improved agreement with available integral observations, but may worsen agreement with unmeasured, and frequently more important, integral design parameters. Advocates of data adjustment or selection respond that differential data are not now and possibly will never be measured to the accuracies required and inferrable from good integral measurements. Other arguments have been put forth on both sides of the controversy. In any case, the strategy chosen by a nuclear design organization to deal with

inadequacies in the nuclear data base is of sufficient consequence that the choice is made deliberately and the resulting adjusted or selected data base often is protected.

Here we suggest an approach 27 having potential not confined solely to the design organization, and we describe a computer program, ALVIN, to implement and test the approach. We assume the existence of an evaluated nuclear data file, specifically ENDF/B, containing carefully analyzed and selected integral data as well as differential data, and containing for these quantities evaluated variance and covariance data as well. The combined first and second moment differential and integral data set, or a particularly significant part of the data set, first is tested for consistency in the statistical chisquared sense. (Consistency tests are discussed in Sec. II-A.) If the data are consistent, there can be no objection to adjusting the differential data to improve agreement of predictions with the integral observations. (Data adjustment is discussed in Sec. II-B.) When consistency has been established, data adjustment is unlikely to distort unrealistically the differential data base. If, on the other hand, the combined differential-integral data set is clearly inconsistent, data adjustment may be questionable and it might be more profitable to use expedients such as design biases until the source of the inconsistency is identified and resolved.

The next step is to identify the source of the inconsistency, and this also is discussed in Sec. II-A. If the inconsistency arises from over-optimism as to the accuracy of integral data, this result is of great interest to designers in treating design biases and margins. More likely there are a number of sources of inconsistency. Consistency tests applied to the unadjusted data set provide details of discrepancies only in particular integral data. For corresponding details of inconsistencies in particular differential data, the necessary techniques are formally the same as data adjustment by least squares. Intuitively, one is looking for critical directions in the combined space of integral and differential parameters for which reduction of the least squares functional forces the point representing the data set to move far beyond reasonable probability. Thus we are led to data adjustment for

analysis of consistency as well as for the achievement of an improved data base.

The ALVIN code provides the computational capability for this approach. Consistency and adjustment procedures used in the code are described in Sec. II, while necessary sensitivity calculations are described in Sec. III. Programming techniques are outlined in Sec. IV, and a code abstract is included as Appendix A. The data consistency and adjustment module, DAFT2, is adapted from a previous code, DAFT1. 28 Sample problems are described in Sec. V and Appendixes C, D, E, and F. Code validation is carried out in terms of the sample problems by carrying out required calculations in distinct ways, then comparing the results. Data for three ZPR assemblies provide the sample problem for the data consistency and adjustment portions of ALVIN. The sample problem for the sensitivity parts of the code is one for which a biological dose equivalent is produced by D-Be neutrons penetrating a thick iron shield. Input and output are described in Sec. VI. Capabilities and limitations of ALVIN are summarized in Sec. VII.

II. CONSISTENCY TESTS AND DATA ADJUSTMENT

Group cross sections, particle and photon yield data, and other differential data in a nuclear data library will be represented by x_1, x_2, \dots, x_{r} , where f, the number of differential parameters, may be of order 103 to 105. Integral parameters y1, y2, ..., y4 such as reactivity worths and reaction rate ratios are computed as functions of the primary parameters $y_{1}(x_{1},x_{2},...,x_{q})$ for i=1,2,...,f, or $y_{1}(x)$ in a convenient notation. Here 1, the number of integral parameters, usually is of order 101 or 102. From a combination of measurements, corrections, and analyses one arrives at "evaluated" observed values x1, $x_2^e, \dots, x_{\hat{1}}^e$ and $y_1^e, y_2^e, \dots, y_{\hat{1}}^e$. Usually the evaluated observed values of the integral parameters do not equal the values of the integral parameters calculated using the evaluated data base x . That is, y

^{*}Other data might include x_j representing a nuclear temperature characteristic of inelastic neutron emission as suggested by D. W. Muir. As another example, x_j might be a mixing parameter such that the cross section is $x_j\sigma_a + (1-x_j)\sigma_b$, where σ_a and σ_b are alternative physically reasonable evaluations of the cross section.

differs from $y_i(x^e)$. In dealing with this discrepancy, we assume that numerical experimentation has shown it to be a result of errors in differential data, or integral data, or both, and not a result of inadequate computational techniques.

A. Tests for Consistency among Differential and Integral Data

The data may be discrepant in that $y_i^e \neq y_i(x^e)$, but at the same time they may be consistent in view of uncertainties in measurement and evaluation. The combined set of differential and integral parameters may be consistent in that their values could reasonably have been drawn from an assigned joint probability distribution. To test for consistency we frame the so-called simple null hypothesis 29 that the populations are normal with the evaluated means, variances, and covariances. We then draw a sample from the population and compute values for one or more statistics. The values thus obtained permit a decision to accept or reject the hypothesis at a certain level of confidence.

Consider initially the quadratic form

$$s_{1} = \sum_{i=1}^{\hat{1}} \sum_{i=1}^{\hat{1}} [y_{i}(x^{e}) - y_{i}^{e}]^{yy} v_{ii}^{-1}$$

$$[y_{i}(x^{e}) - y_{i}^{e}] , \qquad (1)$$

where yy is the evaluated matrix of variances and covariances among the evaluated integral parameters. That is, ${}^{yy}v_{ij}$, represents the evaluated variance of y_i^e if i = i' and the evaluated covariance of y_i^e with y_1^e , if i \neq i'. Under the simple null hypothesis we expect S_1 to be distributed as a $\chi^2_{\hat{i}}$ distribution with 1 degrees of freedom, symbolized as $\chi_{?}^{2}$. Here the values y, (xe) are calculated outside ALVIN and are regarded as sample values from the multivariate normal distribution with means y_i^e and evaluated variance-covariance matrix yy V. For example, for the case described in Sec. V-A, $\hat{\mathbf{1}}$ is 24 and $\mathbf{S}_{\hat{\mathbf{1}}}$ is found to be 503. For the χ^2_{24} distribution the value of 503 is far outside the 1% probability limits (there is a 1% probability that χ^2_{24} is less than 10.7 and a 1% probability that χ^2_{24} exceeds 43.0). Thus the simple null hypothesis is rejected at the "highly significant" level of 1%. We take this to imply that the combined set of means, variances, and covariances for the evaluated parameter set is highly inconsistent.

In practice the integral observations usually are considered to be independent (when common quantities like delayed neutron fraction are removed from quantities like reactivity worth observation). The quadratic form then becomes

$$s_{1} = \sum_{i=1}^{1} [y_{i}(x_{i}^{e}) - y_{i}^{e}]^{2}/yy_{ii}, \qquad (2)$$

where ${}^{yy}v_{ii}$ represents the evaluated variance for the evaluated integral parameter y_i^e . The individual contribution of each integral parameter to the value of S_1 is evident and is distributed as a χ^2_1 distribution with one degree of freedom according to the hypothesis. Thus deviant integral data can be identified under the initial hypothesis. However, no information has been obtained as to the consistency of particular differential data with this procedure.

To examine the consistency of the combined differential and integral data, consider the quadratic form

$$S_2 = \sum_{i=1}^{\hat{1}} \sum_{i=1}^{\hat{1}} [y_i(x) - y_i^e]^{yy} W_{ii}[y_i(x) - y_i^e]$$

$$+ \sum_{j=1}^{\hat{j}} \sum_{j'=1}^{\hat{j}} [x_j - x_j^e]^{xx} W_{jj}, [x_j, - x_j^e]$$

+
$$2\sum_{i=1}^{\hat{1}} \sum_{j=1}^{\hat{j}} [y_i(x) - y_i^e]^{xy} W_{ij}[x_j - x_j^e]$$
 , (3)

subject to the requirements that

$$y_{i}(x) = y_{i}(x^{e}) +$$

$$+ \sum_{j=1}^{\hat{J}} \frac{\partial y_{j}}{\partial x_{j}} \Big|_{x^{e}} [x_{j} - x_{j}^{e}] , i=1,2,...,\hat{I}. (4)$$

The weight matrix W in the quadrature form will be taken to be the inverse of the matrix V of evaluated variances and covariances among the evaluated differential and integral parameters. YW will represent the partition corresponding to the integral parameters, XX will represent that for the differential parameters, and XYW will represent that for both. The matrices V and W are symmetric.

Different samples of differential and integral data will yield differing sample values of S2. At the evaluated point $x = x^e$, used in the preceding initial tests, S_2 resembles S_1 . If we minimize S_2 by adjusting the combined data set to $x = x^a$, then the sample value of S_2 is also distributed as χ_1^2 . We can ask if the data set is consistent after adjustment by examining the new value of S2. In the previous example S2 is found to be 108 but remains improbably large. Data adjustment may be risky in such cases. Nevertheless, we can examine the contribution to S_2 of residuals $x_4^a - x_4^e$ in order to identify potentially deviant differential or integral data. The least squares adjustment process here is looked upon as a device to identify anomalies in the connected network of differential and integral data. Thus we are led to consider data adjustment, both for its role in the strategy of data improvement outlined in Sec. I, and for determination of data consistency.

Before discussing data adjustment it is useful to touch briefly on the normal approximation and on the linearity of Eq. (4).

Our consistency tests assume that the populations are normal, an assumption often made by evaluators in arriving at the evaluated variances and covariances. Hence, the assumed normality and the evaluated data values are related, and it is natural to have them appear together in the consistency tests. Nevertheless, the assumption of normality may be inadequate.

Linear expressions relate calculated integral parameters to differential parameters in Eq. (4) for convenience and because $\partial y_i/\partial x_j$ is easily calculated by perturbation techniques, while higher derivatives are not. The computation of $y_i(x)$ and $\partial y_i/\partial x_j$ is discussed in detail in Sec. III. We note here only that the computation of $\partial y_i/\partial x_j$ for $j=1,2,\ldots,\hat{j}$ is carried out in a single calculation when, as in ALVIN, linear perturbation theory is used for the derivatives.

B. Nuclear Data Adjustment

Many groups have investigated and applied various adjustment techniques to nuclear data. One might, as in other disciplines, introduce cost factors C_1 , which represent the cost to the design of an error in predicting y_1 in the sense that the overall design penalty is a function of the C_1 and of the deviations $|y_1-y_1^e|$ from unknown true values y_1 . In the absence of a more realistic penalty function, the nuclear designer might use differential data sets adjusted to minimize

$$c = \sum_{i=1}^{\hat{1}} c_i |y_i(x) - y_i^e| .$$
 (5)

This strategy, however, does not reflect uncertainties in determination of the differential and integral data. Moreover, it does not respond to the objection that to decrease one set of design biases may increase others for which integral observations are sparse. Most investigators have used a mixed strategy that attempts to improve the basic data set as well as the integral results, or at least does not seriously degrade the differential data. Barré, Chaudat, and others^{3,5} have adjusted the differential data in multigroup form so as to minimize

$$s_1 = \sum_{i=1}^{1} [y_i(x) - y_i^e]^2 / yy_{ii}$$
, (6)

as in Eq. (2), but subject to constraints

$$|x_{j} - x_{j}^{e}| < b_{j}$$
 , j=1,2,..., (7)

Conversely, Cecchini et al. 7 minimize the sum of squared residuals for the differential data,

$$s_2 = \sum_{j=1}^{\hat{J}} [x_j - x_j^e]^2 / x^{x_j}$$
, (8)

subject to constraints

$$|y_i(x) - y_i^e| < a_i$$
, i=1,2,3,...,i . (9)

British, Israeli, and other groups 13,18,21 have minimized the general quadratic form, Eq. (3), assuming

correlations to be negligible, whereas Swedish 10,11,12 and Japanese 15,16 groups and others have included some correlations. It appears that correlations in the differential data 30,31 should be included. 16 Finally, linear programming techniques have been employed to minimize 25

$$S_{3} = \sum_{i=1}^{\hat{1}} \left| y_{i}(x) - y_{i}^{e} \right| / \mu_{i} + \sum_{j=1}^{\hat{j}} \left| x_{j} - x_{j}^{e} \right| / \nu_{j}, (10)$$

subject to constraints

$$|y_{i}(x) - y_{i}^{e}| < \mu_{i}$$
 , i=1,2,..., (11)

and

$$\left|x_{j} - x_{j}^{e}\right| < v_{j}$$
 , $j=1,2,...,\hat{j}$. (12)

Where bounds are required in Eqs. (6)-(12) they are usually taken to be one or two times standard deviations.

We choose to use the least squares approach, minimizing the quadratic form in Eg. (3), because of the connection of this technique with consistency tests. Bounds are not placed on changes of differential data during adjustment. 2,9 When the integral parameters are assumed to be linearly dependent on the differential data, as is expressed in Eq. (4), it is not necessary to iterate to convergence 32 in order to compute adjustments. Thus the data adjustment subroutines DAFT2 and DAFT3 (to be described) are simpler than DAFT1, 28 but their notation and coding techniques are otherwise similar. DAFT2 adjusts data and computes diagnostics in the general case when differential and integral parameters may be correlated; matrices of order at least j x j are inverted in this case. DAFT3 computes the same quantities, but requires inversion only of 1 x 1 matrices by use of a special technique described in Sec. II-B-2. This technique is only applicable when the differential data are uncorrelated with the integral data, but it permits simultaneous adjustment of arbitrarily large differential data libraries.

1. Data Adjustment with Full Correlations --DAFT2. It is convenient conceptually and for coding purposes to form the union of the differential and integral parameters and to normalize them by dividing by their evaluated values. Let

$$z_{k}(x) = \frac{z_{k}}{z_{k}^{e}} = \begin{cases} y_{k}(x)/y_{k}^{e} & \text{for } k=1,2,...,1 \\ x_{k}/x_{k}^{e} & \text{for } k=1+1,1+2,...,1+1=k \end{cases}$$
(13)

Similarly, the primary quantities to be adjusted are transformed to

$$x_{j} = x_{j}/x_{j}^{e}$$
 for j=1,2,..., \hat{j} . (14)

Let ${}^{ZZ}{}^{!}V_{kk}$, represent the evaluated variance for the evaluated parameter z_k^e if k=k', or the evaluated covariance between z_k^e and z_k^e , if $k\neq k'$. Note that

 $ZZ'V_{kk'} = ZZ'V_{kk'}/(z_k^e z_k^e)$. Let ZZ'V represent the matrix with elements $ZZ'V_{kk'}$, and form the weight matrix

$$ZZ'_{W} = ZZ'_{V}^{-1} = \begin{pmatrix} YY_{W} & YX_{W} \\ XY_{W} & XX_{W} \end{pmatrix} .$$
 (15)

This matrix is partitioned only to relate to the partitioned matrices appearing in Eq. (3); DAFT2 makes no assumptions requiring partitioning, such as that YXW vanishes. The Gauss-Markov theorem shows that for this choice of weight matrix, the variances are minimized for any linear combinations of the adjusted parameters; thus the variances on derived integral quantities are minimized as well. When normal distributions are assumed, as is done for our consistency tests, this is a maximum-likelihood estimate as well. ^{29,33}

The quadratic form to be minimized is, from Eq. (3),

$$s_2 = [Z(X) - Z^e]^{tr} ZZ^t w[Z(X) - Z^e]$$
 (16)

Here Z and z^e are column vectors with elements \boldsymbol{z}_k and ones, respectively. The linear relations, Eq. (4), between differential and integral quantities are transformed to

$$z_k(x) = z_k(x^e) + \sum_{j=1}^{\hat{j}} A_{kj}[x_j - x_j^e]$$
,

$$k=1,2,...,\hat{k}$$
 , (17)

where

$$z_{k}(x^{e}) = \begin{cases} y_{k}(x^{e})/y_{k}^{e} & \text{for } k=1,2,...,1\\ 1 & \text{for } k=1+1,...,n \end{cases}, \quad (18)$$

and

$$A_{kj} = \begin{cases} z_{k}(X^{e})D_{kj} \\ & \text{for } k=1,2,\ldots,\hat{1} \text{ and } j=1,2,\ldots,\hat{j} \end{cases}$$

$$\begin{cases} \delta_{j,k-\hat{1}} \\ & \text{for } k=\hat{1}+1,\ldots,\hat{k} \text{ and } j=1,2,\ldots,\hat{j} \end{cases}, (19)$$

and

$$D_{kj} = \frac{x_{j}^{e}}{y_{k}(x^{e})} \frac{\delta y_{k}}{\delta x_{j}} \Big|_{x^{e}}$$
for k=1,2,...,\(\frac{1}{2}\) and j=1,2,...,\(\frac{1}{2}\). (20)

The D matrix is the matrix of computed relative sensitivities. The normal equations to be solved are

$$\sum_{k=1}^{\hat{R}} \sum_{k'=1}^{\hat{R}} [z_k(x^e) - z_k^e + \sum_{j'=1}^{\hat{J}} A_{kj}, (x_j, -x_j^e,)]$$

$$\times {}^{ZZ'}W_{kk^{\dagger}}A_{k^{\dagger}j} = 0$$
 for $j=1,2,...,\hat{j}$, (21)

with solution

$$x_j^a = x_j^e + \sum_{j=1}^{\hat{j}} c_{jj}^{-1}, B_j, \text{ for } j=1,2,...,\hat{j}$$
 (22)

Here

$$B_{j} = \sum_{k=1}^{\hat{k}} \sum_{k'=1}^{\hat{k}} [z_{k}^{e} - z_{k}(x^{e})]^{ZZ'} W_{kk'} A_{k'j}$$
for j=1,2,...,ĵ, (23)

and

from Eq. (17),

$$Y_{1}^{a} = y_{1}^{a}/y_{1}^{e} = y_{1}(x^{e})/y_{1}^{e}$$

This symbolism follows that in DAFT1 and is used in coding DAFT2. Now that the adjusted values of the

differential parameters have been obtained, the asjusted values of the integral parameters develop

$$+\sum_{j=1}^{\hat{J}} A_{ij} [x_j^a - x_j^e] . \qquad (25)$$

The matrix C^{-1} is the matrix of variances and covariances among the adjusted quantities as derived from the input evaluated uncertainty matrix $^{ZZ^{\dagger}}V$, but it does not reflect the actual dispersion in the data. Hence it is customary, 29,33 in obtaining the variance-covariance for the normalized adjusted data, to multiply by $S_2^a/\hat{1}$, a "dispersion multiplier," where S_2^a is computed after adjustment.

$$XX_{M} = \frac{S_{Z}^{a}}{2} c^{-1}$$
 (26)

If S_2^{a}/\hat{T} is less than unity, it is replaced by unity in ALVIN. Similarly, combining Eqs. (25) and (26), one obtains the variance-covariance matrix among the adjusted integral quantities,

$$YY_M = A^{XX_M} A^{tr}$$
 (27)

and the covariance matrix between adjusted integral and differential quantities,

$$\mathbf{Y}\mathbf{X}_{\mathbf{M}} = \mathbf{A}^{\mathbf{X}\mathbf{X}}_{\mathbf{M}} \qquad (28)$$

2. Adjustment of Arbitrarily Large Differential Data Sets -- DAFT3. Daft 2 must invert one matrix (V) of order $(\hat{1} + \hat{j}) \times (\hat{1} + \hat{j})$ and one matrix (C) of order $\hat{j} \times \hat{j}$. When \hat{j} , the number of differential quantities in the library, is large, say 10^3 to 10^5 , the matrix inversion becomes a problem which is frequently resolved by adjusting only part of the data set. Had the adjustment been applied to another

$$c_{jj}^{\dagger} = \sum_{k=1}^{R} \sum_{k'=1}^{R} A_{kj}^{22'} W_{kk'} A_{k'j}^{\dagger} \text{ for } j, j' = 1, 2, ..., \hat{j} .$$
 (24)

part of the library, the result would be different. This matrix inversion problem can be circumvented, 8 and arbitrarily large differential data sets adjusted simultaneously when, as is assumed by most groups, the differential data are uncorrelated with the integral data.

Let ^{YY}V represent the evaluated variance-covariance matrix for the evaluated integral quantities, let ^{XX}V represent the evaluated variance-covariance matrix for the differential quantities, and suppose that the evaluated differential quantities are uncorrelated with the evaluated integral quantities. The weight matrix expressed by Eq. (15) then has partitions $^{YY}W = ^{YY}V^{-1}$, $^{XX}W = ^{XX}V^{-1}$, and $^{XY}W = 0$. Let ^{YX}A represent the upper $\mathbf{\hat{1}} \times \mathbf{\hat{j}}$ partition of the A matrix expressed by Eq. (19). That is, a component $^{YX}A_{kj}$ of this $\mathbf{\hat{1}} \times \mathbf{\hat{j}}$ matrix is $\mathbf{Z}(\mathbf{X}^e)\mathbf{D}_{kj}$. The adjusted values of the differential quantities are obtained in this case from

$$X^a - X^e = XX_V YX_A tr(YY_V + YX_A XX_V YX_A tr)^{-1}$$

$$\times [Y^e - Y(X^e)] , \qquad (29)$$

where the largest matrix to be inverted is only of order $\hat{\mathbf{1}} \times \hat{\mathbf{1}}$. The adjusted values of the integral quantities are obtained as before from Eq. (25). The variance-covariance matrix of the adjusted differential quantities is

$$XX_V^a = XX_V - XX_V YX_A tr(YY_V + YX_A XX_V YX_A tr)^{-1}$$

$$\times {}^{YX}A {}^{XX}V$$
 (30)

and again a matrix of order only $\mathbf{\hat{1}} \times \mathbf{\hat{1}}$ must be inverted. The variance-covariance matrix XX M is obtained from Eq. (26) by replacing C by XX V a , and YY M and YX M are computed as before from Eqs. (27) and (28), respectively.

Because 1 usually is much less than 1, this technique, coded as DAFT3, requires inversion of much smaller matrices than is the case for DAFT2.

III. SENSITIVITY CALCULATIONS

The calculations described in the previous section required derivatives $\delta y_i/\delta x_j$ of integral parameter i with respect to differential parameter j.

These derivatives can be expressed conveniently as relative sensitivities [see Eq. (20)],

$$p_{ij} = \frac{x_j^e}{y_j(x^e)} \frac{\delta y_j}{\delta x_j} \bigg|_{x^e} , \qquad (31)$$

where both integral values $y_i(x^e)$ and derivatives are computed for a given evaluated differential data set x^e . Many workers also have contributed to this development. We now describe computations of relative sensitivities and derived quantities, such as sensitivity profiles, from linear perturbation theory using SENSI and related modules in ALVIN.

A. Inhomogeneous Transport

The particle or photon flux $\psi(\xi)$ at a point ξ in phase-time space satisfies the inhomogeneous linear Boltzmann equation

$$L\psi = S \qquad , \tag{32}$$

where $S(\xi)$ is the local source density. The adjoint flux $\psi^+(\xi)$ satisfies the adjoint equation

$$L^{\dagger}\psi^{\dagger} = S^{\dagger}$$
 , (33)

where $S^+(\xi)$ is an adjoint source, and where L^+ is an operator adjoint to the Boltzmann operator L. The adjoint operator and boundary conditions on ψ^+ are defined such that

$$(\psi^+, L\psi) = (L^+\psi^+, \psi)$$
 (34)

Here (ϕ,χ) symbolizes an inner product, in this case just the integral of $\phi(\xi)\chi(\xi)$ over the relevant region of phase-time space.

Choose $S^+(\xi)$ so that (S^+,ξ) is an integral quantity of interest. Suppose that the operators and sources change as might occur, for example, if differential nuclear data are changed. Then

$$(L + \delta L)(\psi + \delta \psi) = S + \delta S , \qquad (35)$$

and

$$(L^{+} + \delta L^{+})(\psi^{+} + \delta \psi^{+}) = S^{+} + \delta S^{+}$$
 (36)

When these results are combined, it follows that the exact change $\delta(s^+,\psi)$ in the integral quantity, even for large changes in operators and sources, is

$$\delta(s^{+}, \psi) = -(\psi^{+}, \delta L[\psi + \delta \psi]) + (\psi^{+}, \delta s)$$

$$+ (\delta s^{+}, \psi + \delta \psi) \qquad (37)$$

or

$$\delta(s^{+}, \psi) = -(\delta L^{+}[\psi^{+} + \delta \psi^{+}], \psi) + (\psi^{+} + \delta \psi^{+}, \delta s)$$

$$+ (\delta s^{+}, \psi) , \qquad (38)$$

in addition to two other equivalent forms.

We now confine ourselves to the case of fixed sources and small perturbations, i.e., to linear perturbation theory. In this case, from Eqs. (37) and (38),

$$\delta(S^+, \psi) = -(\psi^+, \delta L \psi) = (-\delta L^+ \psi^+, \psi)$$
 (39)

Further, consider the time-independent, one-spacedimensional, multigroup situation for which the Boltzmann equation and its adjoint are

$$(\Omega \cdot \nabla + \Sigma_{\mathbf{g}}) \psi_{\mathbf{g}}(\underline{\mathbf{r}}, \underline{\Omega})$$

$$- \sum_{\mathbf{g}^{\dagger} = 1}^{\hat{\mathbf{g}}} \sum_{\mathbf{j} = 0}^{\infty} \frac{2\mathbf{j} + 1}{4\pi} \Sigma_{\mathbf{g}^{\dagger} \to \mathbf{g}}^{\mathbf{j}} \psi_{\mathbf{g}^{\dagger}, \mathbf{j}}(\underline{\mathbf{r}})^{\mathbf{p}} \mathbf{j}^{(\mu)}$$

$$= S_{\mathbf{g}}(\mathbf{r}, \underline{\Omega}) , \qquad (40)$$

and

$$(-\Omega \cdot \nabla + \Sigma_{\mathbf{g}}) \psi_{\mathbf{g}}^{+}(\underline{\mathbf{r}}, \underline{\Omega})$$

$$- \sum_{\mathbf{g'}=1}^{\hat{\mathbf{g}}} \sum_{\mathbf{j}=0}^{-\infty} \frac{2\mathbf{j}+1}{4\pi} \Sigma_{\mathbf{g}\to\mathbf{g}}^{\mathbf{j}}, \psi_{\mathbf{g'},\mathbf{j}}^{+}(\underline{\mathbf{r}}) P_{\mathbf{j}}(\mu)$$

$$= S_{\mathbf{g}}^{+}(\underline{\mathbf{r}}, \underline{\Omega}) , \qquad (41)$$

for each multigroup g=1,2,..., \hat{g} . Here $\psi_{g}(\underline{r},\underline{\Omega})$ and $\psi^{+}(\underline{r},\underline{\Omega})$ are the adjoint flux, respectively, at posi-

tion \underline{r} in multigroup g and in direction $\underline{\Omega}$, with Legendre expansions

$$\psi_{\mathbf{g}}(\underline{\mathbf{r}},\underline{\Omega}) = \sum_{j=0}^{\infty} \frac{2j+1}{4\pi} \psi_{\mathbf{g}j}(\underline{\mathbf{r}}) P_{j}(\mu) , \qquad (42)$$

$$\psi_{\mathbf{g}}^{+}(\underline{\mathbf{r}},\underline{\Omega}) = \sum_{\mathbf{j}=0}^{\infty} \frac{2\mathbf{j}+\mathbf{1}}{4\pi} \psi_{\mathbf{g}\mathbf{j}}^{+}(\underline{\mathbf{r}}) P_{\mathbf{j}}(\mu) , \qquad (43)$$

in terms of the Legendre polynomials, $P_j(\mu)$, of the polar angle cosine μ . The Legendre coefficients of flux, ψ_{gj} , and adjoint flux ψ_{gj}^+ , are readily computed from S_N , multigroup Monte Carlo, P_N , and diffusion theory solutions, and their use eliminates the necessity for determining consistent quadrature techniques for the inner product, so Legendre fluxes and adjoint fluxes are utilized henceforth. In this case the inner product expressions of Eqs. (37) and (38) become

$$\delta(s^{+}, \psi) = -(\psi^{+}, \delta L \psi)$$

$$= \int d\underline{r} \sum_{\mathbf{g}} \sum_{\mathbf{j}=0}^{\infty} \frac{2\mathbf{j}+1}{4\pi} \psi_{\mathbf{g}\mathbf{j}}^{+}$$

$$\times \left[-\delta \Sigma_{\mathbf{g}} \psi_{\mathbf{g}\mathbf{j}} + \sum_{\mathbf{g}^{+}} \delta \Sigma_{\mathbf{g}^{+} + \mathbf{g}}^{\mathbf{j}} \psi_{\mathbf{g}^{+}\mathbf{j}}\right] , \quad (44)$$

and

$$\delta(s^{+}, \psi) = -(\delta L^{+}\psi^{+}, \psi)$$

$$= \int d\underline{r} \sum_{g} \sum_{j=0}^{\infty} \frac{2j+1}{4\pi}$$

$$\times \left[-\delta \Sigma_{g} \psi_{gj}^{+} + \sum_{g'} \delta \Sigma_{g+g'}^{j}, \psi_{g',j}^{+}\right] \psi_{gj}, \quad (45)$$

for the change in the integral quantity consequent to changes in group cross sections. Thus for changes in

particular cross sections we obtain from either Eq. (14) or (15) the results

$$\frac{\partial (S^+,\psi)}{\partial \Sigma_g} = -\int d\underline{r} \sum_{j=0}^{\infty} \frac{2j+1}{4\pi} \psi_{gj}^+ \psi_{gj}^-, \quad (46)$$

$$\frac{\partial (S^{+}, \psi)}{\partial \Sigma_{g^{+} \rightarrow g}^{j}} = \int d\underline{r} \frac{2\underline{j} + \underline{1}}{4\pi} \psi_{g\underline{j}}^{+} \psi_{g^{+}\underline{j}}^{+} \qquad (47)$$

These derivatives, of the form $\partial y_i/\partial x_i$, completely characterize nuclear data sensitivities as computed by multigroup S_N , Monte Carlo, P_N , or diffusion theory codes. Fission neutron production cross sections can be thought of as being absorbed in the $\Sigma_{g^{1}\rightarrow g}^{j}$ arrays. The expressions, Eqs. (46) and (47), do not require cross sections or values of (S^{\dagger}, ψ) , i.e., y,, so they represent a discrete calculation which is carried out by a basic subroutine, SENSI, in ALVIN. Legendre fluxes and adjoint fluxes are read in (KFLUX=1) by subroutine REDFLX, or are computed (KFLUX=2) by REDFLX from discrete ordinate fluxes and adjoints. SENSI computes the inner product in slab, spherical, or cylindrical geometry according as KGEOM is 1,2, or 3, respectively. In ALVIN the derivative $\partial(S^+,\psi)/\partial\Sigma_g$ is labeled DYDG(IG), and $\partial (S^+, \psi)/\partial \Sigma_{g' \to g}^{j}$ is labeled DYDL(IJ,IGI,IG). These quantities can be normalized and stored into sensitivity arrays for use in data adjustment.

If the inhomogeneous problem is time-dependent, we merely add a time integral to the inner product, add $V_g^{-13\psi}/\partial t$ to Eq. (40), add $-V_g^{-13\psi}/\partial t$ to Eq. (41), and note that these do not change when differential multigroup data are changed. Thus Eqs. (46) and (47) apply also to the time-dependent case if the right-hand sides are integrated over time. If KTIMS = 1, the time integral is carried out in SENSI by reading in fluxes and adjoints at each time step, executing Eqs. (46) and (47), multiplying by the width of the time step, accumulating, and repeating the operation for all time steps.

Two aspects of the adjoint source S⁺ are noteworthy. First, suppose (S⁺, ψ) represents a detector response or dose such that a response or dose per unit monoenergetic flux is $\Sigma_{\rm det}$ over a volume $V_{\rm det}$; then we wish (S⁺, ψ) to equal $V_{\rm det}\Sigma_{\rm det}\psi_0$ if the angle integrated flux ψ_0 is uniform over the detector re-

gion. The inner product (s^+,ψ) then is $\int\!\! d\underline{\Omega} \int\!\! d\underline{r} s^+(\Omega) \psi(\Omega) \text{ or } V_{\text{det}} s^+(\Omega) \psi_0 \text{ in this case. Thus}$ the directed adjoint source $s^+(\Omega)$ is Σ_{det} , but the angle integrated source frequently input into transport codes is $4\pi\Sigma_{\text{det}}$.

Second, consider a time-dependent problem for which the response of interest is the temperature $\theta(t_m)$ at a time t_m , of a material of volume \mathbf{V}_m , with total heat capacity C, with a total heat transfer coefficient K to a reservoir, and subject to fission heating. Let \mathbf{q}_g represent the local energy deposition per fission in group g. Then

$$c\frac{d\theta}{dt} + \kappa\theta = \sum_{g} \int d\underline{r} \int d\underline{\Omega} \ q_{g} \Sigma_{fg} \psi_{g} \qquad (48)$$

The solution to Eq. (48) is

$$(S^+, \psi) = \theta(t)$$

$$= \int_{0}^{t} dt' \sum_{g} \int d\underline{\Omega} \int_{V_{m}} d\underline{r} e^{\frac{\underline{k}c(t-t')}{c} \frac{q_{g}}{c} \Sigma_{fg} \psi(t')}$$
(49)

so the angle-integrated adjoint source is

$$S_g^+ = 4\pi q_g \Sigma_{fg} \frac{1}{c} e^{-\frac{K}{c}(t-t_m)} U(t-t_m)$$
 (50)

in V_m and zero elsewhere. Here we have used the unit function $U(\tau)$ which is unity for $\tau \ge 0$ and is zero otherwise. Adjoint sources generally can be constructed by this method.

B. Reactivity, Rossi-α, and Other Eigenproblems

The transport operator L can be broken up in many ways and for each there is an eigenproblem,

$$L'\psi_{a} = aL'' \psi_{a} . \qquad (51)$$

Here ψ_a is the eigenfunction corresponding to eigenvalue a. For example, L" might be the fission neutron production operator, in which case 1/a is the multiplication factor. For another example, L" might be in multigroup notation a square matrix whose elements are zero except on the main diagonal where the elements are inverse speeds, V_g^{-1} . In this case, a represents the Rossi- α parameter. For any particular breakup of the transport operator, there is a

set of eigenvalues and a corresponding set of eigenfunctions of which ordinarily only one, the fundamental, is real and non-negative. The fundamental is usually the only eigenfunction computed by conventional transport codes.

After nuclear data change, L becomes $L + \delta L$, and the eigenvalues and eigenfunctions change accordingly,

$$(L' + \delta L')(\psi_a + \delta \psi_a)$$

= $(a + \delta a)(L'' + \delta L'')(\psi_a + \delta \psi_a)$. (52)

Subtracting Eq. (51) from Eq. (52) and linearizing, we leave

$$\delta a L'' \psi_a = (L' - a L'') \delta \psi_a + (\delta L' - a \delta L'') \psi_a$$
 (53)

Adjoint to Eq. (51) is the relation

$$L^{i}^{\dagger}\psi_{a}^{\dagger} = aL^{ii}^{\dagger}\psi_{a}^{\dagger}$$
 (54)

with the adjoint boundary conditions described earlier. Multiply Eq. (53) by ψ_a^+ and integrate over phase space. The first terms on the right-hand side of Eq. (53) contribute nothing in view of the adjoint property expressed in Eq. (31), with the result that

$$\delta \mathbf{a} = \frac{(\psi_{\mathbf{a}}^{\dagger}, [\delta L' - a\delta L'']\psi_{\mathbf{a}})}{(\psi_{\mathbf{a}}^{\dagger}, L''\psi_{\mathbf{a}})} . \tag{55}$$

The fundamental eigenvalue is an integral quantity of considerable interest and according to Eq. (55) its change can be computed using only the fundamental eigenfunction and adjoint. A much more difficult situation arises when the integral quantity of interest is a ratio of reaction rates

$$R_{rq} = \frac{(s_r^+, \psi_a)}{(s_n^+, \psi_a)}$$
 (56)

both measured in the fundamental flux. In this case

$$\frac{\delta R_{rq}}{R_{rq}} = \frac{(s_r^+/R_{rq} - s_q^+, \delta \psi_a)}{(s_q^+, \psi_a)} , \qquad (57)$$

and an inner product with $\delta\psi_{\bf a}$ is required. Often in mathematical physics when an eigenfunction change is required it is expanded in a complete set of eigenfunctions. In the transport problem, however, we are unlikely to have available any eigenfunctions other than the fundamental.

Usachev⁴⁴ has developed an iterative algorithm for computation of Eq. (57) requiring repeated solution of the inhomogeneous transport equation. We develop an alternative algorithm and suggest its use in an appropriate way that only requires knowledge of the unperturbed flux and adjoint. Let $\psi_{\mathbf{r}}^{+}$ represent the solution to the inhomogeneous equation,

$$L^{i}^{\dagger} \psi_{r}^{\dagger} = S_{r}^{\dagger} . {(58)}$$

Insert this expression into Eq. (57) and apply the adjoint property, Eq. (54). Then

$$\delta R_{rq} = \frac{(\psi_r^+/R_{rq} - \psi_q^+, L'\delta\psi_a)}{(S_q^+, \psi_a)}$$
 (59)

The linearized Eq. (52) can be rearranged to provide an iterative calculation of the nth approximation, $\delta\psi_{a,n}\text{, to the desired }\delta\psi_{a}\text{,}$

$$L'\delta\psi_{a,n} = (a\delta L'' + \delta a L'' - \delta L')\psi_a$$

+ $aL''\delta\psi_{a,n-1}$, (60)

with starting condition $\delta\psi_{a,0}=0$. This constitutes an algorithm for computation of the required $L^{\dagger}\delta\psi_{a,n}$ under proper conditions of convergence. Here we terminate at n=1, whereupon, approximately,

$$\delta R_{rq} = \frac{(\psi_r^+/R_{rq} - \psi_q^+, [a\delta L'' + \delta a L'' - \delta L']\psi_a)}{(S_q^+, \psi_a)}. (61)$$

The above approximation is not coded into this version of ALVIN.

Returning to the eigenvalue perturbations, we now apply the previously described techniques to develop the inner products in Eq. (55) for Rossi- α and for reactivity perturbations. For Rossi- α ,

$$\frac{\partial \alpha}{\partial \Sigma_{g}} = -\frac{1}{D_{\alpha}} \int d\underline{\mathbf{r}} \sum_{j}^{\infty} \frac{2j+1}{4\pi} \psi_{\alpha gj}^{\dagger} \psi_{\alpha gj}$$
 (62)

and

$$\frac{\partial \alpha}{\partial \Sigma_{g^{\dagger} \to g}^{j}} = \frac{1}{D_{\alpha}} \int d\underline{r} \frac{2\underline{j}+1}{4\pi} \psi_{\alpha g \underline{j}}^{\dagger} \psi_{\alpha g^{\dagger} \underline{j}} , \qquad (63)$$

where

$$D_{\alpha} = \int d\underline{r} \sum_{g} \sum_{j}^{\infty} \frac{2j+1}{4} \psi_{\alpha gj}^{+} \frac{1}{V_{g}} \psi_{\alpha gj}$$
 (64)

For reactivity perturbations, it is convenient to break up $\Sigma_{g^1 \to g}^j$ into a scattering portion and a fission portion

$$\Sigma_{g'\to g}^{j} = \Sigma_{g'\to g}^{sj} + \nu_{g'}\Sigma_{fg'}\chi_{g'\to g}\delta_{jo} . \qquad (65)$$

Then,

$$\frac{\partial \rho}{\partial \Sigma_{g}} = -\frac{1}{D_{\rho}} \int d\underline{r} \sum_{i}^{\infty} \frac{2\underline{j+1}}{4\pi} \psi_{\rho g j}^{+} \psi_{\rho g j}^{-} , \qquad (66)$$

and

$$\frac{\partial \rho}{\partial [\Sigma_{\mathbf{g'+g}}^{\mathbf{sj}} + (1-\rho) \nu_{\mathbf{g'}} \Sigma_{\mathbf{g'}} \chi_{\mathbf{g'+g}} \delta_{\mathbf{jo}}]}$$

$$= \frac{1}{D_{\rho}} \int d\underline{r} \sum_{g} \frac{2j+1}{4\pi} \psi_{\rho g j}^{+} \psi_{\rho g' j}^{-} , \qquad (67)$$

where

$$D_{\rho} = \int d\underline{r} \sum_{g} \sum_{g'} \psi_{\rho g 0}^{+} \frac{v_{g'}}{4\pi} \Sigma_{f g'} \chi_{g' \to g} \psi_{\rho g' 0}. \quad (68)$$

These expressions also are in their simplest form.

Equations for sensitivities thus far have been expressed as derivatives with respect to macroscopic cross sections. Ordinarily a sensitivity of interest will be for a single material or nuclide, but this may occur with different number densitities DENS(IR) in different spatial regions IR=1,2,...,NR. A derivative with respect to a microscopic cross section σ is obtained from the corresponding derivative with respect to a macroscopic cross section Σ as in Eqs. (46), (47), (62), (63), (66), and (67) by

$$\frac{\partial}{\partial \sigma} = \sum_{IR=1}^{NR} \int_{\substack{\text{Region IR}}} \frac{d\mathbf{r} \text{ DENS(IR)* remainder of }}{\text{expression}}$$
 (69)

When sensitivity integrals are coded in SENSI, the number density of the material of interest is included as in Eq. (69) with one exception: The reactivity denominator in Eq. (68) requires the actual macroscopic fission cross sections for the assembly, so these are read in for each group and region and used as macroscopic quantities.

C. Sensitivity Profile

Expressions were developed in the previous sections for derivatives $\partial y/\partial \Sigma_g$ and $\partial y/\partial \Sigma_{g'\to g}$, where y is an integral parameter. These constitute the basic building blocks for compounding derivatives with respect to any differential data, e.g., the inelastic scattering cross sections for 238 U. We illustrate the compounding process not for a particular differential cross section, but for the "sensitivity profile," an interesting parameter characterizing a class of cross-section changes. 43,45

Suppose that for a particular nuclide, say ^{238}U , we change the total cross section in group g by the amount $\delta\Sigma_g^{\text{X}}$, corresponding to a change in reaction x, say an inelastic cross section. The group-to-group transfer cross sections for this reaction, Σ_g^{Jx} , change accordingly, and we make the particular assumption that

$$\frac{\delta \Sigma_{g \to g}^{jx}}{\Sigma_{g \to g}^{j}} = \frac{\delta \Sigma_{g}^{x}}{\Sigma_{g}^{x}} , \qquad (70)$$

for all exit groups g' and for all Legendre orders j.

Cross sections for particle transfer into group g are unchanged. Then, compounding changes by the usual $(\delta_y = \sum_i \frac{\partial y}{\partial x_i} \delta x_i)$ method we have, from Eqs. (46) and (47),

$$\frac{\delta(S^+,\psi)}{(S^+,\psi)} = P_g^{x} \frac{\delta \Sigma_g^{x}}{\Sigma_g^{x}} , \qquad (71)$$

where the sensitivity profile P_g^X is

$$P_g^x = \frac{1}{(s^+, \psi)} \int d\underline{x} \sum_{j=0}^{\infty} \frac{2j+1}{4\pi}$$

$$\times \left[-\Sigma_{\mathbf{g}}^{\mathbf{x}} \psi_{\mathbf{g}\mathbf{j}}^{+} + \sum_{\mathbf{g}'} \Sigma_{\mathbf{g}+\mathbf{g}'}^{\mathbf{j}\mathbf{x}} \psi_{\mathbf{g}',\mathbf{j}}^{+}\right] \psi_{\mathbf{g}\mathbf{j}} \quad . \tag{72}$$

This inhomogeneous sensitivity profile characterizes certain interesting cross-section changes and is computed by subroutine PROFIL in ALVIN.

Similar profiles can be defined and computed for Rossi- α and for reactivity and in general under other assumptions than Eq. (70), but we do not carry these out in ALVIN.

Bartine et al. 45 use the definition Eq. (71) for inhomogeneous sensitivity profile, but they appear to state, on the basis of equations like Eqs. (34) and (39), that another definition can be used,

$$P_g^{x'} = \frac{1}{(s^+, \psi)} \int d\underline{r} \sum_{j=0}^{\infty} \frac{2j+1}{4\pi} \psi_{gj}^+$$

$$\times \left[-\Sigma_{g}^{x} \psi_{gj} + \sum_{g'} \Sigma_{g'+g}^{jx} \psi_{g'j}\right] \qquad (73)$$

In paraphrase, because $(\psi^+,\delta L\psi)$ equals $(\delta L^+\psi^+,\psi)$, then $\psi^+\delta L\psi$ equals $\psi\delta L^+\psi^+$ over some more limited region of phase space. There is no a priori reason to expect this to be generally true, although it is true for the fully absorptive case. We have devel-oped a complete analytic solution to the case of hydrogenous slowing down in an infinite homogeneous medium to be used in clarifying a variety of problems. For this case the two definitions of P_x^x are

not equal and, because our definition, Eq. (71), was arrived at by the orderly process of compounding, we believe it it correct.

IV. ALVIN PROGRAMMING

ALVIN is programmed in FORTRAN-IV to be machine-independent except for large storage requirements which, in the distributed version, are specific to the CDC-7600. Five large arrays are stored in LCM and only a few statement lines would need to be changed for other machines. Otherwise, specific CDC features are avoided, e.g., Hollerith is used for formatting rather than asterisks. A code abstract is included as Appendix A.

The code consists of the main ALVIN routine and eight principal subroutines with about 1100 statement lines, approximately 20% of which are comment lines. The routines, the subroutines they call, and their tape requirements are listed in Table I. A subroutine SENRD2, which generates sensitivities specific to a sample problem, is provided as well. Sensitivity and variance-covariance matrices are so large, and so frequently have integral regularities, that it may be useful to create subroutines like SENRD2 to generate them for specific problems.

Program variables have the same significance in all parts of the code, and their values, with a few exceptions, are passed through labeled commons. All variables are defined in Appendix B, and these definitions hold in all parts of ALVIN. Certain systematics have been followed in variable naming.

TABLE I

ROUTINE CALLS AND TAPE REQUIREMENTS IN ALVIN

Routine	Calls or Requires
ALVIN	SENSRD (SENRD2), SENSI, DAFT2, DAFT3
SENSRD	
SENSI	REDFLX, CROSEF, CROSEC, PROFIL
REDFLX	Flux tape, adjoint flux tape
PROFIL	
CROSEF	
CROSEC	Cross section tape
DAFT2	INFO, MATINV
DAFT3	INFO, MATINV
INFO	
MATINV	

For example, indices have a fixed meaning, and temporaries are formed by suffix T. Variable names usually are similar to notation used in Secs. II and III describing the calculations.

The structure of ALVIN is shown in Fig. 1.

Pairs of control parameters KSENS and KADJST define various modes of code operation. For example, KSENS=3 and KADJST=2 result in sensitivities being read in by SENSRD, some sensitivities being calculated and added by SENSI, and consistency tests and data adjustment being carried out for full correlation by DAFT2. A simple case is KSENS=1 and KADJST=1 where sensitivities are calculated by SENSI, and no data adjustment or consistency calculations are carried out.

V. SAMPLE PROBLEMS AND CODE VALIDATION

Two sample problems are provided, one stressing the data consistency and adjustment parts of ALVIN, and one stressing the sensitivity parts of the code. The sample problems are used to illustrate capability, input, and output. In addition, however, the sample problems are used to validate the code by carrying out the same calculation in different ways.

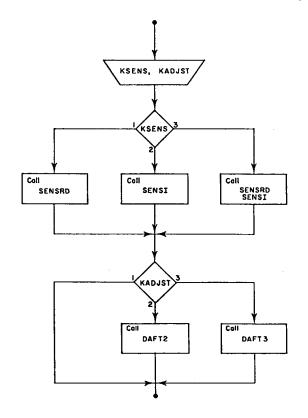


Fig. 1. ALVIN structure.

A. Data Consistency and Adjustment

Integral observations made on LMFBR-like criticals have frequently failed to agree with calculations. Reactivity worths in particular have been discrepant, thus presenting the nuclear designer with serious problems in view of the importance of reactivity worths in the design process. Data for three important criticals, ZPR-6-6A, ZPR-6-7, and ZPR-3-48, prominently display the reactivity worth discrepancy and have been compactly presented by Bohn. 47 Table II identifies 24 integral parameters $y_1, i=1,2...,24$, for these assemblies, and Table III identifies 19 differential nuclear quantities x_4 , j=1,2...,19, of interest. It is convenient to allow y_{\downarrow} to represent the ratio of the computed value C_{\downarrow} of an integral parameter to its experimental value $\mathbf{E_i}$, and to let $\mathbf{x_i}$ represent the ratio of the nuclear datum σ_j to its evaluated value σ_j^e . Then the evaluated quantities y_1^e and x_j^e are unity, and

$$\frac{\partial y_{\underline{i}}}{\partial x_{\underline{j}}}\Big|_{x} = \left(\frac{\sigma_{\underline{j}}}{c_{\underline{i}}} \frac{\partial c_{\underline{i}}}{\partial \sigma_{\underline{j}}}\right)\Big|_{x} = -\left(\frac{\sigma_{\underline{j}}}{E_{\underline{i}}} \frac{\partial E_{\underline{i}}}{\partial \sigma_{\underline{j}}}\right)\Big|_{x} = . \quad (74)$$

This normalization is essentially that described in Sec. II-B-1. The effects of cross-section changes on inference of E, from experiment are made explicit in Eq. (66). For i=1,2,3 the integral parameters are the C/E values for multiplication factors of ZPR-6-6A, SPR-6-7, and ZPR-3-48, indicated in the second column of Table II by subscripts A, 7, and 8, respectively. For i=4,5...,15 the integral parameters are the C/E values for central worths of 239 Pu, 235 U, 238 U, and 10 B, indicated by 49, 25, 28, and B, respectively, as superscripts on W; for example, the C/E value for the central worth of 239 Pu in the ZPR-6-7 assembly is indicated by W_7^{49} in Table II. Finally, for i greater than 15, the integral parameters y, are C/E values of ratios of reaction rates, e.g., $^{1}_{7}^{28c}_{49f}$ for $y_{20}^{}$ represents the C/E value of the 238 U capture rate relative to the 239 Pu fission rate measured in ZPR-6-7. If y, is $(\sigma_n/\sigma_m)/(\sigma_n/\sigma)_E$, then to first order (unchanged flux spectrum),

$$\frac{\partial y_{i}}{\partial x_{j}}\Big|_{x} = \delta_{nj} - \delta_{mj} . \qquad (75)$$

TABLE II

INTEGRAL PARAMETERS y_1 AND VALUES $y_1(x^e)$ COMPUTED USING EVALUATED NUCLEAR DATA PARAMETERS x_1^e [If no adjustment were necessary $y_1(x^e)$ would = unity]

TABLE III PRIMARY NUCLEAR DATA PARAMETERS $\mathbf{x_{i}}$, THEIR UNCERTAINTIES, AND THEIR ADJUSTED VALUES

1	y ₁	y _i (x ^e)	y _i Adjusted	y ₁ Selected	_1_	_ <u>*j</u> _	x ^e	x _j Adjusted by Alvin	x _j Selected by Bohn
1	k _A	0.9920+0.004	by ALVIN 0.993	by Bohn	1	$\sigma_{\mathtt{f}}^{\mathtt{25}}$	1 <u>+</u> 0.1	0.978	0.93
2	k ₇	1.0024 <u>+</u> 0.004	1.001		2	σ <mark>25</mark>	1 <u>+</u> 0.1	0.932	
3	^k 8	0.9927 <u>+</u> 0.004	1.002		3	σ _f 49	1 <u>+</u> 0.1	0.995	0.97
4	w ⁴⁹	1.10±0.025	0.990	1.06	4	σ ⁴⁹	1 <u>+</u> 0.1	0.989	
5	w_{A}^{25}	1.15 <u>+</u> 0.025	1.014	1.05	5	σ ²⁸	1 <u>+</u> 0.15	0.961	0.88
6	w_{A}^{28}	1.24 <u>+</u> 0.035	1.090	1.09	6	σ _f 28	1+0.1	0.979	0.97
7	$w_{\mathbf{A}}^{\mathbf{B}}$	0.92 <u>+</u> 0.075	0.854	0.96	7	σ ²⁸ inel	1 <u>+</u> 0.15	0.840	0.88
8	w ⁴⁹	1.25 <u>+</u> 0.035	1.052	1.14	8	o ^{Na} el	_ 1 <u>+</u> 0.1	1.059	
9	w ₇ 25	1.24 <u>+</u> 0.035	1.036	1.08	9	₀ 0	1±0.1	1.063	
10	w ₇ ²⁸	1.16 <u>+</u> 0.025	0.936	0.95	10	el σ ^{fe} c	1 <u>+</u> 0.1	0.979	
11	w <mark>B</mark>	1.18 <u>+</u> 0.035	1.027	1.17	11	σ σ c	_ 1 <u>+</u> 0.1	1.001	
12	w ₈ ⁴⁹	1.25 <u>+</u> 0.035	1.042	1.12	12	ς σ <mark>Cr</mark>	_ 1 <u>+</u> 0.1	0.995	
13	w ₈ ²⁵	1.26 <u>+</u> 0.035	1.046	1.08	13	c v _d 28	_ 1 <u>+</u> 0.06	1.138	1.10
14	w ₈ ²⁸	1.27 <u>+</u> 0.035	1.024	0.99	14	α ν _d 25	- 1 <u>+</u> 0.04	1.106	1.012
15	w ^B 8	1.09 <u>+</u> 0.035	0.960	1.06	15	√49 Vd	1 <u>+</u> 0.06	1.166	1.024
16	A ^R 25f	0.90 <u>+</u> 0.03	0.942		16	√40 √d	1±0.1	1.009	1.016
17	AR ^{28c}	1.03 <u>+</u> 0.03	1.060		17	\(\frac{1}{\nu_d^{41}}\)	1 <u>+</u> 0.1	1.009	
18	7 ^R 49f	0.99 <u>+</u> 0.02	0.975		18	g ^{Na}	1 <u>+</u> 0.1	0.995	
19	7 ^R 49f	1.05+0.02	1.032		19	o ^C el	1 <u>+</u> 0.1	1,085	
	7 ^R 49f	-				el	- <u></u>		
20	7 49£	1.09+0.02	1.053		The	third co	lumns of Tabl	les II and III l	ist the val-

The third columns of Tables II and III list the values of the parameters determined at the evaluated point together with standard errors, most of them assigned by Bohn, for the quantities. Most of the computed reactivity worths, y₄ through y₁₅, are high and differ from unity by many standard errors; this is the reactivity worth discrepancy. Uncertainties in reactivity worths due to uncertainties in delayed neutron yields are not included, because the delayed data (j=13,17) are assigned uncertainties and

24

21

22

7^R25f

7^R25f

8^R25f

0.94+0.02

1.04+0.02

0.96+0.05

0.94+0.05

0.924

1.023

0.961

0.924

TABLE IV SENSITIVITY COEFFICIENTS $(x_j/y_i) \partial y_i/\partial x_j$ FOR ZPR-6-6A, ZPR-6-7, AND ZPR-3-48 (REF. 47)

		· · · · · · · · · · · · · · · · · · ·								
		(I,J),J=1,MJ	_ a	-0.	8 0000F_0 2	-2 7000F-01	-3.0000E-02	-0.	-0.	→0 .
1	. •	-1.0000E-01		-0.	-0.	-Ø.	-0,	+0.	-0.	•••
_	-0.	-0.	-0.	-7.0000E-02	A AGGGF-G2		-6,0000E-02		-0.	-0.
2	-0.	-0.	_		-0.	-0.	-0,	-0.	-0.	- •
_	-0.	-0.	-0.	-0, 			-7,0000E-02		-0.	-0.
5	-0.	-0.	_	-6.0000E-02			-0.	-0.	-0.	-•
	-0.	-0.	-0.	-0.	-0.	-0.	4 7000E-02	-4 5000F-02	-1.1500E-01	2 0000F-03
4	-9,9100E-01	4.40005-02	1.10005+00	-1.01005-01	-6 34005-01	-4-22005-01		-5.0000E-03		£ 4 0 5 11 0 £ 1 0 2
_			-1.4400E-01		-2 04005-01	⇒0. 2 10005_91	-0, * ***********************************	-2 1000E-02	-2,7000E-02	1 00005-02
5	2.6490E-01	-1./4MUE-01	-0.	-0.	-2.0600E+01	_		4.0000E-03		
			-1.4400E-01		-U. -E 9700E-01	-0.	-0. 3.4600E-01			-1 4888F-82
6	-1.3450E+0U	-9,40001-02	₹ 0.	•0.		1.225ØE+90		2.0000E-03		-1,4000
_			-1.4400E-91		-N.	-0.	-0. 2.0800E-01		2,1300E-01	-2 98995-82
7	-1.2520E+00			-0.		-9.2000E-02		2.0000E-02		#C.0000C-0C
			-1.4400E-01	ומ-שממטכים	**************************************	-0,	-0,			2 0000E_02
8	-0,	-0.	2,1300E-01	-8.30001-02	-4,1/000-01	1,44000-01	1,1100E-01	-4,7000E-02	-0	3,00005-03
	-3.0000E-03	-2.0000E-03	-3.2600E-W1	-2.52NUL-U2	-7.9/WNE-WI	-2,0000E-02	-3.1200E-02	-1,0000E-03	7 FAGAE_43	0 80005-03
9	1.1790E+00	-1.9000E-01	-1.1010E+00	5. DUNUE-UZ	-5,4100E-01	1.5/005-01	1,700000-01	4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4	- a 2	A. 0000C-03
	3.0000E-03	4.000UE-03	-3.2600E-01	-2.5200E-02	-5.9/NUE-NI	-2.0000E-02	-3.1200E-02	0. NOUSE - 03	1 02005 01	. 2 GGGGE-02
10	-0.	-0.	-1.2070E+00	-1.2100E-01	-7.7800E-01	1.04501+00	4.9000E-01		1.9200E-01	-5 * NADAE -05
	3.0000E-03	-3.0000E-03	-3.2600E-01	-2.5200E-02	-5.9700E-01	-2.0600E-05	-3.1200E-02	1,000000	-V.	. 7 70005 . 03
11	-0.	-0.	-1,1290E+00	-2.1600E+01	-5.0900E-01	-2.6000E-01	2,8300E-01		3.1600E-01	+2+3000C+0C
	4.0000E-03	-4.0000E+03	-3,2600E-01	-2,5200E-02	-5.9700E-01	-2.0600E+05	-3.1200E-02	2,00006-03	***	+ 00005 07
12	-0.	-0.	2.4700E-01	-6.9000E-02	-4.650UE+01	2.1100E-01	1.4400E-01	-9.0000E-03	-V.	1,0000E-03
	-3,000UE-03	-2.0000E-03	-3.5600E-01	-2.1000E-02	-5.9900E-01	-1.2100E-92	-1,2100E-02	-2.NNNNE-N3	-6.00005-02	/ 0000F 07
13	1.1990E+00	-2.1400E-01	-1.0740E+00	6.8000E-02	-4.1700E-01	1.6200E+01	1,8300E-01	-2,0000E-03	-0,	6.0000E-03
	2.0000E-03	3,0000E-03	~3.5600E-01	-2.1000E-02	-5,9900E-01	-1.5100E-05	-1.5100E-05	3,0000E-03	5.7000E-02	4 3000- 03
14	-0.	-0.	-1.4460E+00	-1.6700E-01	-1.0260E+00	1.2730E+00	6.4000E-01	4.7000E-02		-1.2000E-02
	-0.	-4.0000E-03	-3.5600E-01	-2,1000E-02	-5.9900E-01	-1.2100E-02	-1.2100E-02	-1,0000E-03	3.9500E-01	4 0000 00
15	-0.	-0.	-1.1990E+90	-2.7300E+01	-5.6100E-81	-2,2600E-01	3,3800E=01	N,5000E-02	-0.	-1,8000E-02
	1.0000E-03	-4.0000E-03	-3.5600E-01	-2.1000E-02	-5.9900E-01	-1.2100E-02	-1.2100E-02	+Ø.	5.1700E-01	_
16	_	-1.0000E+00		0.	0.	1.0000E+00	0.	0.	0.	0,
	0.	0.	0.	0,	0.	0.	0.	0,	0.	_
17		-1.0000E+00	0.	0.	1.0000E+00	θ,	€.	Ø.,	0,	0,
	0.	0.	0.	Ø,	0.	0,	0.	0.	0,	_
18		0.	-1.0000E+00	0.	я.	1.0000E+0U	0.	0,	0.	0.
	0.	0.	0.	0.	0,	0,	0.	-0.	0.	_
19	1.0000E+00	0.	-1.0000E+00	0.	Ø.	0.	0,	0,	0,	0,
•	0.	Ø.	0.	Ø.	0.	a,	0.	Ø,	0,	_
28		0.	-1.0000E+00	0.	1.0000E+00	0.	0.	0.	0,	0,
	Ø.	Ø.	0.	ø <u>.</u>	Ø.	0.	ø.	0,	0.	
21	-1.000UE+00	0.	0.	0.	1.0000E+00	И.	0.	0,	ø.	0,
	A.	0.	0.	ø.	Ø.	8	0.	0,	0.	
22	-1.0000E+00	ø.	ø.	Ø.	1.0000E+00	-	0.	0.	0.	Ø.
	9.	9.	ő.	ø.	0.	0	0.	0,	0.	
22	-1.0000E+00	0.	ő.	0.	ø.	1.0000E+00	0.	0,	0	0.
د ع	0.	0.	ø.	0.	0.	Й.	0.	0.	0.	
3/1	-1.0000E+00	Ø.	0.	0.	1.0000E+00	ศ.	ø.	0.	0.	Ø,
£ 4	N.	9.	0.	0.	0.	0.	0.	0.	ø,	

examined separately. 48 The uncertainties ascribed to differential data in Table III assume that cross-section errors are correlated at all energies. Sensitivities presented by Bohn are listed in Table IV. Calculated results shown in Tables I through III used ENDF/B-III as the evaluated data base as processed into multigroup form by SDX. Values of differential and integral parameters adjusted by ALVIN also are listed in Tables II and III and show physically plausible trends. Values selected by Bohn from six trial sets of differential quantities also are listed. Our data adjustments are intended to be illustrative only of the techniques involved and, particularly, illustrative of consistency inferences. More detailed study of data uncertainties and sensitivities would be required to justify an adjusted data set for nuclear design application.

Input for this sample problem is shown in Appendix C. The output, shown in Appendix D, provides considerably more information, particularly consistency information, than do Tables II through IV. Values of chi-squared before and after adjustment both are improbably large, 503 and 91, respectively, for 24 degrees of freedom. The dispersion multiplier DISPR is 3.8 for this problem, thus accounting for the fact that errors in the adjusted data in Tables II and III are larger than input evaluated errors in many cases. Contributions of the 43 differential and integral parameters to chi-squared are listed before and after adjustment.

This sample problem is not fully illustrative of the capabilities of DAFT3 in that many more than 19 differential data could be treated by DAFT3. However, the sample problem is useful for code validation in that, with only 24 + 19 parameters, data adjustment can be carried out by DAFT2 as well as by DAFT3. To facilitate this comparison, inputs to DAFT2 and DAFT3 are made similar when only standard error information is provided. DAFT2 and DAFT3 results agree for this problem, thus validating the consistency and data adjustment part of the code.

Sensitivity Calculation

Illustrative of sensitivity calculations in ALVIN is a spherical representation of a thick iron shield-collimator. 49 The shield consists of a 70cm-radius sphere of iron with a 4-cm-radius void at the center. An isotropic neutron source is uniformly distributed in a central 1-cm-radius sphere with the 0° spectrum of neutrons produced by 50-MeV deuterons

on beryllium. 50 The response quantity consists of the product of the neutron flux and neutron fluenceto-dose equivalent conversion factor summed over all neutron energy groups and averaged over the volume of the 1-cm-thick air shell at the outer surface of the sphere.

The S_N transport code DTF⁵¹ was used to calculate the neutron fluxes and adjoint fluxes throughout the shield, using 41-group, P-5 cross sections and S-16 quadrature. The source for the adjoint calculation, located in the 1-cm-thick shell surrounding the sphere, was the vector of neutron fluence-to-dose equivalent conversion factor.

Directed fluxes and adjoint fluxes were read in to ALVIN through REDFLX and converted to Legendre components. Nuclear data were read in through CROSEC and CROSEF. Fluxes and nuclear data were used by SENSI to compute detailed sensitivities as described in Sec. III-A. These were then used by PROFIL to compute sensitivity profiles as described in Sec. III-C. The computed sensitivity profile as a function of energy group is illustrated in Appendix E and output is listed in Appendix F.

All routines in ALVIN that are concerned with sensitivity are used in calculation of the sensitivity profile, and can be validated by a direct calculation. The sensitivity profile P(IG) represents the change in neutron dose-equivalent rate at the shield surface resulting from a change in cross section in group IG combined with proportionate changes in transfer cross sections from group IG to other groups. The ALVIN calculation uses first-order perturbation theory; this approximation, as well as code accuracy, can be validated by comparison with direct calculations.

The direct approach to determine the change in the result due to a change in the cross-section data involves the creation of an altered cross-section set, performing a neutron transport calculation using the altered cross sections, and converting the fluxes in the outer shell to the neutron dose equivalent rate. The fractional change in the dose equivalent rate divided by the fractional change in the cross sections of group IG thus yields the sensitivity P(IG) of the result to cross sections in group IG.

Sixteen separate, altered cross-section sets were formed with $\Sigma_{\pi}(IG)$ and $\Sigma^{j}(IG \rightarrow IG')$, IG' = IG,NGfor all j increased by 0.1, 0.5, 1.0 or 10.0% for

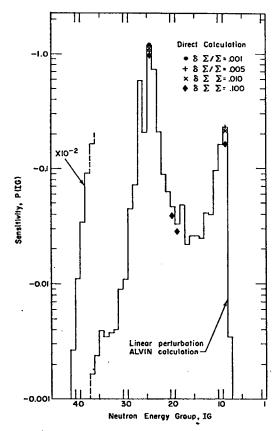


Fig. 2. Sensitivity of shield surface neutron dose-equivalent rate to neutron cross-section data computed by direct change in cross sections and by linear perturbation -- ALVIN calculation.

group IG = 9, 19, 20, or 25. The sensitivities resulting from the neutron transport calculation are superimposed on the sensitivity profile histogram of Fig. 2. The separate DTF calculations were converged to 10^{-4} , so the only directly calculated sensitivities shown are those for which the relative change in dose equivalent exceeded 10^{-4} . For example, the dose equivalent changed from 0.7189 x 10^{-13} rem/s to 0.7188 x 10^{-13} , 0.7187 x 10^{-13} , and 0.7186 x 10^{-13} rem/s, when the cross sections of group 19 were increased by 0.1, 0.5, and 1.0%, respectively. Therefore, these cases were disregarded.

In addition to accuracy problems in the direct calculation, there are nonlinearity problems in the perturbation calculation. Consider monoenergetic neutron penetration through a slab of thickness X with cross section Σ . Then,

$${}^{P}_{\text{direct}} = -\left[1 - \frac{1}{2!} \times \Sigma \frac{\delta \Sigma}{\Sigma} + \frac{1}{3!} (\times \Sigma \frac{\delta \Sigma}{\Sigma})^{2} - \dots\right] \times \Sigma . (76)$$

If $\delta\Sigma/\Sigma$ is chosen to be 0.1 to insure accuracy in the dose equivalent change, then for the shield thickness studied here (about 12 mean free paths thick) the direct calculation underpredicts the result for very small $\delta\Sigma/\Sigma$ by about one-third according to Eq. (75). An underprediction of this order of magnitude can be observed in Fig. 2 for the direct calculation with $\delta\Sigma/\Sigma$ equal to 0.1. Conversely one can conclude from these results that linear perturbation theory will overpredict the change in dose equivalent by about one-third when fractional changes of 10% in cross section are considered.

Useful direct calculations for the purpose of validating ALVIN's linear perturbation calculations should have $\delta\Sigma/\Sigma$ sufficiently small to avoid the nonlinear effects discussed above and sufficiently large to avoid inaccuracy problems. The results shown in Fig. 2 are in good agreement and are believed to validate the inhomogeneous sensitivity parts of ALVIN. Calculations of sensitivities for Rossi- α and reactivity utilize inhomogeneous sensitivities and have not been validated separately.

VI. INPUT AND OUTPUT

Input requirements are shown in Table V. Formats and precise variable descriptions are given in terms of the variable definitions listed in Appendix B.

Outputs are labeled also by variable name and follow the examples shown in Appendixes D and F.

VII. SUMMARY OF ALVIN CAPABILITIES AND LIMITATIONS

ALVIN carries out sensitivity calculations for steady-state or time-dependent inhomogeneous transport. For eigenproblems, ALVIN computes sensitivities of eigenvalues to nuclear data changes (specifically reactivity and Rossi-α), but does not compute sensitivities of eigenfunction properties such as reaction rate ratios. Sensitivities are computed with respect to total cross section, with respect to individual Legendre components of group-to-group transfer cross sections, and with respect to fission parameters. Sensitivity profiles are computed.

ALVIN carries out data consistency and adjustment calculations for arbitrary variances and covariances among the differential and integral data. DAFT2 is used for these calculations and the number of parameters treated is limited by the necessity for in-

TABLE V

ALVIN PROBLEM INPUT

(KSENS=1, KADJST=3, KVAR=2)

Order	Format	Contents
1	16A5	Title
2	1216	KSENS, KADJST, MI, MJ
3	16A5	Title
4	6E12.6	DYDX(I,J),J=1,MJ A card set for each I=1,MI.
5	16A5	Title
6	6E12.6	YC(I), I=1,MI
7	16A5	Title
8	1216	KVAR
9	6E12.6	VE(R1,K2),K2=1,MK A card set for each K1=1,MK.

version of large matrices. The DAFT3 subroutine carries out data consistency calculations and adjusts an arbitrarily large and correlated differential base uncorrelated with integral data. Least squares techniques are employed throughout. Limits on data adjustments are not used in ALVIN.

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The authors are grateful to R. J. LaBauve, D. W. Muir, M. Becker, and M. G. Stamatelatos for many pleasant and fruitful discussions on various aspects of this work. We also are grateful to E. M. Bohn for advice on data for the ZPR sample problem and to J. Y. Barré, J. B. Smathers, and W. E. Davey for useful discussions on the methodology.

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APPENDIX A

PROGRAM ABSTRACT

- 1. Name of program: ALVIN.
- 2. Name of computer for which program is designed: CDC-7600.
 - Programming Language: FORTRAN-IV.
- 3. Nature of the problem solved: ALVIN analyzes the consistency of a set of differential and integral nuclear data, adjusts the differential nuclear data to improve agreement with integral observations, and identifies inconsistent data. ALVIN also computes required sensitivities and related quantities such as sensitivity profiles.
- Method of solution: Linear perturbation theory is used for sensitivity calculations. Data consistency and adjustment computations use least squares techniques.
- 5. Restrictions on the complexity of the problem:

 The DAFT2 consistency and adjustment subroutine treats fully or partially correlated differential and integral parameters, but only as many as the order of the largest matrix that can be inverted. The DAFT3 consistency and adjustment subroutine treats arbitrarily large differential data sets, but only if they are uncorrelated with the integral data.
- 6. Related and auxiliary programs: None.

- Typical running times: About 1 min, depending on size of problem.
- 8. <u>Description</u>: Equations, calculational methods, input and output are described in Ref. 1.
- Unusual features: Data set consistency is analyzed. A special algorithm is used in DAFT3 to treat arbitrarily large data sets.
- 10. Status: The program is currently in use and can be obtained from the Argonne Code Center.
- 11. Machine requirements: Distributed version uses
 LCM to store five large arrays. Otherwise machine-independent.
- 12. Operating system: Independent.
- 13. Other programming information: None.
- 14. References:
 - (1) D. R. Harris, W. A. Reupke, and W. B. Wilson, "Consistency Among Differential Nuclear Data and Integral Observations -- the ALVIN Code for Data Adjustment, for Sensitivity Calculations, and for Identification of Inconsistent Data," Los Alamos Scientific Laboratory report LA-5987 (1975).

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APPENDIX B

DEFINITIONS OF VARIABLES USED IN ALVIN

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DEFINITIONS
    A(11,12)=TEMPORARY MATRIX USED WITH DIFFERENT DEFINITIONS IN DIFFERENT
         SUBROUTINES
    B(J)=VECTOR SOURCE TO REARRANGED NORMAL EQUATIONS
    C(J1, J2) = MATRIX WHOSE INVERSE IS THE ADJUSTED VARIANCE-COVARIANCE MATRIX
         OF INDEPENDENT QUANTITIES. LATER THE INVERSE IS STORED IN C
    CHI2F=CHI-SQUARED AFTER ADJUSTMENT USING EVALUATED SECOND MOMENTS
    CHIZI=CHI-SQUARED INITIAL
    CHIDA=DIAGONAL PART OF CHIZA
    CHIDF DIAGONAL PART OF CHI2F
    CHIDI=DIAGONAL PART OF CHIZI
    DENOMARDENOMINATOR OF D(ALPHA)/D(CROSS SECTION) RELATION
    DENOMR = DENOMINATOR OF D(REACTIVITY)/D(CRUSS SECTION) RELATION
    DENS(IR) = NUMBER DENSITY IN REGION IR
    DETERM=DETERMINANT OF A MATRIX
    DISPRIDISPERSION MULTIPLIER
    DYDG(IG) = DERIVATIVE OF INTEGRAL QUANTITY WITH RESPECT TO TOTAL CROSS
         SECTION IN MULTIGROUP IG
    DYDL(IL, IG1, IG) = DERIVATIVE OF INTEGRAL QUANTITY WITH RESPECT TO IL-1 TH
         LEGENDRE ORDER CROSS SECTION FOR TRANSFER FROM MULTIGROUP IG1 TO
         MULTIGROUP IG
    DYDX(I,J)=DERIVATIVE OF INTEGRAL QUANTITY I WITH RESPECT TO DIFFERENTIAL
         QUANTITY J COMPUTED AT THE EVALUATED DATA POINT
    FLAXL(IM, IL, IG) = IL-1 TH LEGENDRE COMPONENT OF ADJOINT FLUX AVERAGED OVER
          SPACE MESH INTERVAL IM, IN ENERGY GROUP IG
    FLUXL(IM, IL, IG) = IL-1 TH LEGENDRE COMPONENT OF FLUX AVERAGED OVER SPACE
          MESH INTERVAL IM, IN ENERGY GROUP IG
    IA=GUADRATURE ANGLE INDEX
    IDG(ISAVE)=IG INDEX OF SAVED SENSITIVITY CASE
    IDG1(TSAVE)=IG1 INDEX OF SAVED SENSITIVITY CASE
     IDL(ISAVE)=IL INDEX OF SAVED SENSITIVITY CASE
     IDX(ISAVE) = IX INDEX OF SAVED SENSITIVITY CASE
     IDY(ISAVE)=IY INDEX OF SAVED SENSITIVITY CASE IG=MULTIGROUP INDEX
     IL=LEGENDRE ORDER INDEX
     IM=SPATIAL MESH INDEX
     IMMAX(IR)=MESH POINT WITH HIGHEST INDEX IN REGION IR
     IMMIN(IR)=MESH PUINT WITH LOWEST INDEX IN REGION IR
     INDEX(I, J) = TEMPORARY ARRAY USED IN MATRIX INVERSION
     IPIVOT(1)=1EMPORARY ARRAY USED IN MATRIX INVERSION
     IPOS=POSITION OF CROSS SECTION IN OTF CROSS SECTION FORMAT
     IR=REGION INDEX
     IT=TIME INTERVAL INDEX
     ITAPE= FILE SFT NUMBER (1 UR 2)
     ITYPE=TYPE OF SAVED SENSITIVITY CASE, =1 IF INHOMOGENEOUS
          SENSITIVITY, =2 IF D(ALPHA)/D(CHOSS SECTION) SENSITIVITY,
          #3 IF D(REACTIVITY)/D(CHOSS SECTION) SENSITIVITY
     IYR=INDEX OF CASE OF SENSITIVITIES CALCULATED FROM FLUXES AND
          ADJOINT FLUXES READ IN
     JTAPE=ASSIGNED TAPE NUMBER
     KADJST=2 IF DIFFERENTIAL DATA ARE TO BE ADJUSTED USING DAFT2, =3 IF
     DIFFERENTIAL DATA ARE TO BE ADJUSTED USING DAFT3, =1 OTHERWISE KFLUX=1 IF LEGENDRE FLUXES ARE READ IN, =2 IF DIRECTED FLUXES ARE READ IN
          FROM WHICH LEGENDRE FLUXES ARE COMPUTED FOR USE IN SENSITIVITY
          CALCULATIONS
     KTYPE TYPE OF SENSITIVITY CALCULATION, #0 IF INHOMOGENEOUS
          SENSITIVITY, =1 IF D(EIGENVALUE)/D(CROSS SECTION)
     KGEOM=1 IF GEOMETRY IN SENSITIVITY COMPUTATIONS IS SLAB, =2 IF SPHERICAL.
          =3 IF CYLINDRICAL
     KRILX=CONTROL SET IN CODE, =1 IF FLUXES ARE BEING PROCESSED,=2 IF ADJOINT
          FLUXES ARE BEING PROCESSED
     KSENS=1 IF SENSITIVITIES ARE ONLY READ IN, =2 IF SENSITIVITIES ARE ONLY
          COMPUTED FROM INPUT FLUXES AND ADJOINT FLUXES, =3 IF SENSITIVITIES
          ARE BOTH READ IN AND COMPUTED
     KTIMS=1 IF TIME DEPFNDENT FLUXES ARE USED IN SENSITIVITY COMPUTATION
     KVAR=1 IF EVALUATED STANDARD ERRORS ONLY ARE READ IN FOR DIFFERENTIAL AND
          INTEGRAL PARAMETERS, =2 IF FULL EVALUATED VARIANCE-COVARIANCE ARRAY
```

IS READ IN FOR DIFFERENTIAL -INTEGRAL PARAMETERS

APPENDIX B (cont)

```
MI=NUMBER OF INTEGRAL PARAMETERS
MJENUMBER OF DIFFERENTIAL PARAMETERS
MK=MI+MJ=NUMBER OF INTEGRAL-DIFFERENTIAL PARAMETERS
NAENUMBER OF QUADRATURE ANGLES FOR DIRECTED FLUX
NG=NUMBER OF MULTIGROUPS
NL=NUMBER OF LEGENDRE FLUX ORDERS USED IN SENSITIVITY COMPUTATION
NLR=NUMBER OF LEGENDRE FLUX ORDERS READ IN
NLCX=NUMBER OF LEGENDRE CROSS SECTION ORDERS READ IN
NM=NUMBER OF MESH INTERVALS IN SENSITIVITY CALCULATION
NR=NUMBER OF REGIONS IN SENSITIVITY CALCULATIONS
NSAVE=NUMBER OF CASES OF COMPUTED SENSITIVITIES SAVED INTO DYDX
     (IY, IX) MATRIX FOR CASE IYR
NT=NUMBER OF TIME INTERVALS IN SENSITIVITY COMPUTATION
NXR=NUMBER OF IYR CASES FOR WHICH NEW SET OF UN-NORMALIZED
     FVALUATED DIFFERENTIAL PARAMETERS ARE TO BE READ IN AND USED
     FOR SENSITIVITY NORMALIZATION OR PROFILE CALCULATION
NYR=NUMBER OF CASES FOR WHICH FLUXES AND ADJOINT FLUXES ARE READ IN AND
     SENSITIVITIES COMPUTED
P(IG) = SENSITIVITY PROFILE FOR GROUP IG
PIVOT(I)=TEMPORARY ARRAY USED IN MATRIX INVERSION
GCOSA(IA)=COSINE OF QUADRATURE ANGLE NUMBER IA FOR DIRECTED FLUX
QLEGP(IL, IA) = LEGENDRE POLYNOMIAL OF ORDER IL-1 OF QCOSA(IA)
QHTSA(IA) #WEIGHT FOR QUADRATURE ANGLE NUMBER IA
R#RESPONSE, INTEGRATED OVER APPROPRIATE VOLUME OF PHASE SPACE,
     USED IN INHOMOGENEOUS SENSITIVITY NORMALIZATION AND PROFILE
     CALCULATION
RELXE=(XE(J)-XE(J))/SX(J)
RELXF=(XA(J)=XE(J))/SX(J)
RELYE=(YC(I)-YE(I))/SY(I)
RELYF=(YA(I)=YE(I))/SY(J)
RM(IM) = LEFT = HAND COORDINATE OF MESH INTERVAL IM
SIGFN(IG, IR) = MACROSCOPIC FISSION CROSS SECTION IN GROUP IG IN REGION IR
     TIMES FISSION NEUTRON YIELD
SIGTO(IG) *MICROSCOPIC TOTAL CROSS SECTION IN GROUP IG
SIGTR(IG, IG2, IL) *MICROSCOPIC IL-1 TH LEGENDRE COMPONENT CROSS SECTION FOR
     TRANSFER FORM GROUP IG TO GROUP IG2
SORF(IG2) = NORMALIZED FISSION NEUTRON SPECTRUM INTO GROUP IG2
SPDS(IG)=PARTICLE SPEEDS IN GROUP IG
SX(J)=EVALUATED STANDARD ERROR FOR DIFFERENTIAL PARAMETER J
SXA(J)=STANDARD ERROR OF DIFFERENTIAL PARAMETER J AFTER ADJUSTMENT
SY(I) = EVALUATED STANDARD ERROR FOR INTEGRAL PARAMETER I
SYA(I)=STANDARD ERROR OF INTEGRAL PARAMETER I AFTER ADJUSTMENT
TEMSTO(IG, IPOS) = TEMSTO(IM, IA) = TEMPORARY STORAGE FOR CROSS SECTIONS AND FOR
     DIRECTED FLUXES AND ADJOINT FLUXES
TITLE=DESCRIPTIVE TITLE FOR JOB AND FOR SUBSECTIONS OF INPUT
TM(IT) #LOWER BOUND OF TIME INTERVAL IT
VE(K1, K2) = EVALUATED VARIANCE-COVARIANCE VALUE FOR INTEGRAL-DIFFFRENTIAL
     PARAMETERS K1 AND K2. LATER THE INVERSE, IE, WEIGHT MATRIX, IS
     STORED IN VE
VZ(K1,K2) = COMPUTED VARIANCE-COVARIANCE VALUE FOR INTEGRAL-DIFFERENTIAL
     PARAMETERS K1 AND K2 AFTER ADJUSTMENT. INCLUDES DISPERSION FACTOR
     LATER THE ADJUSTED CORRELATION COEFFICIENT MATRIX IS STORED
      IN VZ.
XA(J) * ADJUSTED VALUE OF DIFFERENTIAL PARAMETER J
XE(J) = EVALUATED VALUE OF DIFFERENTIAL PARAMETER J
YA(1) = ADJUSTED VALUE OF INTEGRAL PARAMETER I
YC(I)=VALUE OF INTEGRAL PARAMETER I COMPUTED FOR EVALUATED VALUES OF
      DIFFERENTIAL PARAMETERS
YCU(ISAVE) = VALUE OF INTEGRAL PARAMETER, UN-NORMALIZED, COMPUTED
     FROM EVALUATED DIFFERENTIAL PARAMETERS, USED TO NORMALIZE
      SAVED SENSITIVITY CASE ISAVE. YOU'R IF ITYPE=1,
     #EIGENVALUE IF ITYPE=2,3
YE(I) = EVALUATED VALUE OF INTEGRAL PARAMETER I
 ZA(K)=ADJUSTED VALUE OF INTEGRAL-DIFFERENTIAL PARAMETER
 ZC(K)=VALUE OF INTEGRAL-DIFFERENTIAL PARAMETER K COMPUTED FOR EVALUATED
      VALUES OF DIFFERENTIAL PARAMETERS
 ZE(K)=EVALUATED VALUE OF INTEGRAL-DIFFERENTIAL PARAMETER K
```

APPENDIX C
SAMPLE INPUT FOR DATA CONSISTENCY AND ADJUSTMENT PROBLEM

SAMPLE PROBLEM -- CONSISTENCY AND ADJUSTMENT OF ZPR DATA 2 24 19 1 SENSITIVITIES FOR ZPR PROBLEM .61 -.27 -,1 . Ø8 -.03 .08 -.07 -.26 .66 -.06 -.21 .66 -. 86 .09 **-**,07 -,239 -,991 -,255 .049 1,169 -,161 .047 -.045 -.115 .002 -,906 +,003 -.005 -,856 -,144 , 264 -,206 .210 -.174 .010 .005 .002 -.027 .088 -.024 . 094 -.144 -.856 1,225 -.583 -.094 -1.345 - 002 -.014 .346 .043 .148 .002 -.144 -.856 .002 -.892 -,329 -1.252 -,143 .288 .098 .213 -.020 .004 -. 993 .002 -.856 -. 144 -,083 .199 .213 -.417 -.003 -.002 -, 952 .111 -.027 .003 -.0252 -.597 -, 0296 -.0312 -. 001 -,326 ,050 .137 1.179 -.190 -1,101 -,391 .150 .035 .094 -.004 .009 .003 996 -,0252 -.597 -.0206 -.0312 -.326 -1,207 -.121 -.778 1.045 ,490 .003 -,003 -.020 .192 . 864 .001 -,0312 -.326 -. M252 -.597 -. 0206 -,26A +.509 -1.129 -.216 .283 .316 -,033 .149 .004 -.004 -,0252 -.326 -.597 -.0206 -. 0312 500 .247 -. 869 -.465 .211 -.889 .144 . 661 -,003 -,002 -,002 -.0121 -.0121 -.599 -. 356 -.0210 -.060 -.417 .068 .162 -1.874 -.214 1.199 ,183 -.002 . 406 . 002 .003 .003 -.0121 -,356 -.599 -.0121 -.0210 .057 -1.026 1.273 -1.446 -,167 -.004 .047 .640 -.012 -,356 -.001 -.0210 -,599 -.0121 -.0121 .395 -,273 -.226 -1.199 -,561

-.018

.001

-. 004

,338

. 885

APPENDIX C (cont)

356	 0210	- ,599	0121	0121	
.517		-	•	<u> </u>	
	METERS COMPUT	ED FROM EVAL	LUATED DIFF P	ARAMETERS	
.9920	.9924	.9927	1.10	1.15	1.24
92	1.25	1.24	1.16	1.18	1.25
1.26	1.27	1.09	90	1.03	99
1.05	1.09	94	1.04	.96	.94
		RORS	• • •	• .	•
1					
. 1	, 1	.1	. 1	.15	. 1
.15	. 1	. 1	. 1	. 1	. 1
. 06	.04	.06	. 1	. 1	. 1
. 1		•	-	•	-
.004	.004	.004	.10	.10	.11
15	.11	.11	. 10	.11	.11
.11	.11	.11	.03	.03	.02
.02	.02	.02	.02	.05	.05

APPENDIX D

SAMPLE OUTPUT FOR DATA CONSISTENCY AND ADJUSTMENT PROBLEM

SAMPLE PROBLEM--CONSISTENCY AND AUJUSTMENT OF ZPR DATA

KSENS KADJST MI MJ 1 2 24 19

XE(J), J=1, MJ

.100000E+01 .10000E+01 .100

.100000E+01 .100000E+01

INT PARAMETERS COMPUTED FROM EVALUATED DIFF PARAMETERS

YC(I),I=1,MT
.992000E+M0 .992400E+00 .992700E+00 .110000E+01 .115000E+01 .124000E+01 .920000E+00 .125000E+01 .124000E+01 .116000E+01
.118000E+01 .125000E+01 .126000E+01 .127000E+01 .109000E+01 .900000E+01 .99000E+01 .99000E+01 .105000E+01 .109000E+01
.940000E+00 .104000E+01 .960000E+00 .940000E+00

EVALUATED STANDARD ERRORS

KVAR 1

SX(J), J=1, MJ.100000E+00 .100000E+00 .100000E+00 .150000E+00 .150000E+00 .150000E+00 .100000E+00 .10000E+00 .1000E+00 .10000E+00 .1

\$\text{SY(I),I=1,MI}\$
.400000E-02 .400000E-02 .250000E-01 .250000E-01 .350000E-01 .300000E-01 .300000E-01 .200000E-01 .200000E-01 .200000E-01 .200000E-01 .300000E-01 .30000E-01 .3000E-01 .3000E-01 .3000E-01 .3000E-01 .3

CHIZI REDUCED CHIZI .502816E+03 .209507E+02

CHI2F REDUCED CHI2F DISPR .909101E+02 .378792E+01 .378792E+01

J1 C(J1, J2), J2=1, M.T ADJUSTED VARIANCE-COVARIANCE MATRIX FOR DIFFERENTIAL PARAMETERS 1 .393000 3 .30280 3 .30280 3 .30280 3 .30280 3 .30280 3 .302800 3 .30280 3 20-3671.e. 60-36118P. 61-36256. 30-3168P. 60-3168P. 60-3628P. 60-3628P. 60-3628P. 60-368P. 60-368P. 60-368P. -.15532E-04 -.32287E-04 -.18038E-03 -.35898E-03 -.92722E-04 -.13283E-04 -.23313E-04 -.18213E-04 .56812E-03 3 .25874F-M3 .36940E-M3 .4M24HE-M3 .14441E-M2 .3M219E-M3 .2924E-M3 .14274E-M2 .46M53E-M3 .19556E-M3 -.87850E-M4 -.11442E-M4 .53326F-M4 .53326F-4 23897E-03 .94594E-03 ,14041E-02 .15014F-01 .66660E-03 .84932E-04 .14592E-02 .37128E-02 .37128E-02 .37128E-02 -.95899E-04 -.31761F-03 -.10704E-02 -.41659E-03 -.10206E-02 -.27923E-03 -.40203E-03 -.22302E-03 .55436F-02 5 .34884E-03 .74244E-03 .38219E-03 .66668E-03 .75934E-03 .74244E-03 .74244E-03 .38219E-03 .74244E-03 .74244E-03 .74244E-03 .74244E-03 .75934E-03 .75934E-03 .74244E-03 .7424E-03 . -.23697E-04 -.29190E-04 -.46581E-04 -.10078E-03 -.39015E-04 -.12250E-04 -.24738E-04 -.25140E-04 .25053E-03 6-21775-E-03 .62745E-03 .62745E-03 .62745E-03 .62745E-04 .4072E-04 .4072E-03 .63346E-03 .7233EE-03 .3581WE-03 .17752E-03 -.32456E-04 -.50774E-04 -.93753E-04 -.13663E-03 -.10175E-03 -.18212E-04 -.33731E-04 -.42966E-04 .68404E-03 7 91392E-03 .95461E-02 .41686E-02 .14592E-02 .14645E-02 .63386E-03 .17805E-01 -.1214VE-02 -.41686E-02 .79177E-03 -03010E-05 .24027E-03 .20775E-02 .14763E-02 .26456E-02 .1790E-03 .21705E-03 .12722E-03 -46036E-02 8 .36286E-03 .46053E-03 .32224E-02 .38947E-03 .72330E-03 .34360E-01 -.74250E-02 .71742E-03 -,17371E-03 .445A9E-04 -,40292E-03 -,6451E-03 -,26154E-03 -,11092E-04 -,66451E-05 -,95450E-04 -,1331NF-02 9 .58895E-04 .48116E-03 .19556E-03 .3712ME-02 .13340E-03 .35810E-03 .41686E-02 -.7425ME-02 .17849E-02 .14710E-02 .49185E-03 -.14881E-04 -.59456E-03 -.73158E-03 .23854E-03 .53637E-03 .34969E-03 .58588E-02 10 -.96503E-04 -.13553E-03 -.07017E-04 -.11368E-02 -.91498E-04 -.17752E-03 .79177E-03 .71742E-03 .14718E-02 .37640E-01 -.19516E-05 -.60749E-04 .1913UE-03 .16344E-03 .20452E-03 .41692E-05 -.48996E-05 -.31191E-04 -.53671E-04 11 -.29495E-04 -.15532E-04 -.11842F-04 -.95899E-04 -.23697E-04 -.32056E-04 -.63610E-05 -.17371E-03 -.49185E-03 -.19516E-05 -.37848E-01 -.23942E-04 -.85828E-05 -.34616E-05 -.32114E-06 -.60124E-05 -.31852E-04 -.31805E-04 -.99540E-04 12 -.3552NE-P4 -.322R7E-P4 -.17145E-P4 -.31761E-P3 -.2919NE-04 -.50774E-94 .24027E-05 .44589E-P4 -.14881E-P4 -.60749E-04 --23942E-04 .37845E-01 .49446E-04 .68367E-04 .44881E-04 .43771E-05 .67399E-05 -.31660E-04 -.42454E-04 13 .66727E-04 -.1038E-03 -.5326E-04 -.10744E-02 -.48581E-04 -.93753E-04 -.20775E-02 -.40292E-03 -.59256E-04 -.10138E-03 -,85828E-85 ,49446F-04 ,18575F-01 -,12833E-02 -,45013E-02 -,37780E-03 -,37355E-03 ,48250E-04 -,23989E-03 14 -.75741E-M4 -.35898E-M3 .73756E-M4 -.41659F-M3 -.10778E-M3 -.1386E-M3 -.73158E-M3 .73158E-M3 -.73158E-M3 .14763E-M3 -.34616E-M3 -.73158E-M3 .16344E-M3 -.34616E-M3 -.50849E-M4 -.82559F-M3 .16344E-M3 -.34616E-M3 -.50849E-M4 -.82559F-M3 204525-03 -.927225-04 -.19265-05 -.19265-02 -.398155-04 -.101755-03 -.264565-02 -.261545-03 -.254215-04 -.204525-03 .32114E-06 .440A1E-04 -.45413E-02 .10203E-02 .40199E-02 -.70393E-03 -.96359E-03 .70374E-04 -.71723E-03 16 .46379E-05 -.13283E-04 -.17148E-04 -.27923E-03 -.12250E-04 -.18212E-04 .17986E-03 -.11092E-04 .23854E-03 .41692E-05 .6A124E-A5 .43771E-A5 -.3A78AF-A3 .7A696E-A4 -.7A393E-A3 .37776E-A1 -.1A29AE-A3 .13916E-A4 -.43763E-A3 17 -.30984F-06 -.23313E-04 -.38662E-04 -.49283F-03 -.24738F-04 -.33731E-04 .21705E-03 -.66451F-05 .53637E-03 -.48996E-05 .13452E-04 .67399E-05 -.37355E-03 .67306E-04 -.96359E-03 -.18290E-03 .37536E-01 .26280E-04 -.9384E-03 18 -.3218/E-84 -.18213E-84 -.14335E-84 -.22382E-83 -.2519NE-84 -.4296/E-89 ..12722E-83 -.9545NE-84 -.34969E-83 -.31191E-84 -.31805E-04 -.31660E-04 .40250E-04 .50849E-04 .70374E-04 .13916E-04 .2028E-04 .37841E-01 -.93775E-04 90-13262F-93 .5612E-93 .50-38F-93 .564P4E-93 .684P4E-93 .684P4E-93 .684P4E-93 .56812E-93 .56812E-93 .56812E-93 -.9954BE-84 -.42454E-84 -.23989E-83 -.82559E-83 -.71723E-83 -.43763E-83 -.9384E-83 -.93775E-84 .12598E-81

APPENDIX D (cont)

K1 V7(K1,K2), K2=1,M1 ADJUSTED VARIANCE-COVARIANCE HATRIX FOR INTEGRAL PARAMETERS 1 .44650E-04 .49H3HE-05 .27325F-05 -.55321E-04 .51449E-04 -.4RH85E-04 -.20766E-04 -.41715E-04 .53821F-04 -.24668F-05 -.72616E-05 -.32650F-04 .63293E-04 .21654F-05 -.13811E-04 -.65803E-05 .57399E-04 -.36825E-04 .52471E-04 .28167E-04 -.22683E-04 -.25096E-04 -.83682E-04 -.22683E-04 2 .49638E-05 .28231E-04 .26709F-04 .30977E-04 -.12666E-04 -.16559E-04 -.21776E-04 .18360E-04 -.36012E-04 .78293E-05 16156E-04 .20491F-04 - 40486E-04 .23272E-05 .83385E-05 -.77859E-05 .27750E-05 -.21711E-04 -.15977E-04 -.11538E-04 .43529F-05 .48159E-05 -.64459F-05 .43529E-05 3 .27325E-05 .26509E-04 ,31128E-04 -.63411E-05 .23907E-05 .55745E-05 -.39354E-04 .32121E-04 -.10466E-04 -.65423E-05 -.30712E-04 .28894E-04 -.10600E-04 -.63212E-05 -.16471E-04 .10614E-04 -.16294E-04 .19480E-04 -.16439E-04 -.86505E-05 .68991E-05 .76330E-05 .53554E-04 .68991E-05 4 -,35321E-04 .30977F-04 -.63411E-05 .12476E-02 .62436E-03 .31730E-03 .48955E-03 .25528E-03 -.11437E-03 -.27736E-03 164119E-04 .17288E-03 -.13241E-03 -.96550E-04 .33267E-03 -.12792E-03 .28922E-04 -.20689E-03 -.43244E-04 -.42251E-04 .22772E-05 .25195E-05 -.16108E-03 .22772E-05 5 .51449E-04 -,12666E-04 .23907E-05 .62436E-03 .93843E-03 .80184E-03 .43883E-03 .21118E-04 .18117E-03 .37849E-04 -.25117E-03 -.7647BE-06 .20474E-03 .34374E-04 -.1159BE-03 .49B22E-04 -.99172E-05 .13545E-03 .12050E-03 .78303E-04 -. 40351E-04 -. 44643E-04 .21177F-04 -. 40351E-04 6 -.48885-04 -.16559F-04 .55745E-05 .3173NE-03 .80184E-03 .19471E-02 .10457E-02 -.36279E-03 -.23616E-03 .59643E-03 .7379NE-04 -.15386E-03 -.20012F-03 .44722E-03 -.58596E-03 .27877E-03 .10893E-03 .42956E-04 -.21959E-03 -.17585E-03 4563NE-04 .57484E-04 .24242E-03 .4563NE-04 7 -.20766E-04 -.21776F-04 -.39354F-04 .48955E-03 .43883E-03 .10457E-02 .17354E-02 -.40765E-03 -.64823E-04 -.38327E-04 12978E-02 -.24232E-03 -.12782E-03 -.62251E-03 .43637E-03 .10166E-04 .31023E-03 -.46107E-03 -.24783E-03 -.19165E-03 .56592E-84 .62613E-84 -.22051E-83 .56592F-84 8--41713E-N4 ,1836NE-N4 .32121F-N4 .27528F-03 .21118E-N4-.36279E-N3 -.4N765E-N3 .1N8M9E-N2 .75274E-N3 .2M635E-N3 .72701E-04 .66984E-04 -.5257NE-04 .58874E-04 -.89684E-04 -.71936E-04 -.52178E-04 .99725E-03 .75776E-03 .12969E-03 .18252E-04 .20194F-04 .13909E-03 .18252E-04 9 .53821E-04 -.36012E-04 -.10466E-04 -.11437E-03 .18117E-03 -.23616E-03 -.64823E-04 -.75274E-03 .10496E-04 -.3 31377E-03 .73209E-03 .98964E-03 -.12141E-03 .8623NE-04 .66455E-04 .71696E-04 .77082E-04 .28667E-04 -,44285E-04 -,48996E-04 -,95170E-06 -,44285E-04 10 -.24668E-05 .78293E-05 -.65423E-05 -.20736E-03 -.37849E-04 .59643E-03 -.38327E-04 .20635E-03 .20183E-03 .12389E-02 .6445UE-03 .42515E-03 .12389E-03 .81085E-03 -.3601UE-03 -.18794E-04 -.5694BE-04 .75573E-04 .48321E-04 .45782E-04 -. 38456E-05 -. 42547E-05 . 29193E-04 -. 38456E-05 0.000 -.34808E-04 -.38511E-04 -.30181E-03 -.34808E-04 12 -.32650E-04 .20491E-04 .20893E-04 .17208E-03 -.76478E-06 -.15306E-03 -.24232E-03 .99725E-03 ,73209E-03 .42515E-03 15406E-03 .10H29E-02 .74499E-03 .90429E-05 -.27344E-03 -.92847E-06 -.53403E-04 -.4962E-04 -.13289E-03 -.11002E-03 .24085E-04 .26647E-04 .73380E-04 .24085E-04 13 .63293E-04 -.49496F-04 -.10688F-04 -.13241E-03 .20478E-03 -.20812E-03 .75776E-03 .98964E-03 .12389E-03 .72125E-05 .74499F-03 .11078F-02 .21752E-03 .23881E-03 .61885E-04 .68163E-04 -.11999E-04 .77933E-05 -.15928E-04 - 20713E-04 - 22917E-04 - 18673E-04 - 20713F-04 14 .21654E-05 .23272E-05 -.63212E-05 -.96550E-04 .34374E-04 .44722F-03 -.6251E-03 .12969E-03 -.12141E-03 .810A5E-03 -.68563E-03 .90429E-05 .21752E-03 .27809E-02 .11767E-02 .29784E-04 -.62848E-04 .66816E-04 -.79498E-05 -.29616E-04 -.17942E-04 15 -.13611E-04 .83385E-05 -.16471E-04 .33267E-03 -.11598E-03 -.59596E-03 .43637E-03 .72701E-04 .86230E-04 -.36010E-03 .89472E-03 -.27344E-03 .23881E-05 .11767E-02 .27883E-02 -.57204E-04 .11126E-03 -.12767E-03 .47294E-04 .46455E-04

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-. 22775E-05 -. 25198E-05 -. 16704E-03 -. 27775E-05
16 -.65803E-05 -.77859F-05 .10614F-04 -.12792F-03 .49822E-04 .27877E-03 .10166E-04 .66984E-04 .66455E-04 -.18794E-04 .7879E-04 .66984E-04 .66984E-04 .66984E-04 .66984E-04 .78794E-04 .7879
      -.12344E-03 -.13657E-03 .44999E-03 -.12344E-03
17 .57399E-04 .27750F-05 -.16294E-04 .28922E-04 -.99172E-05 .10893E-03 .31023E-03 -.52570E-04 .28551E-04 -.56948E-04
        .11062E-03 -.53403F-04 .68163E-09 -.6280HE-04 .11126E-03 .13235E-02 .17651E-02 -.15491E-03 .94442E-04
        .26037E-03 .28807E-03 .32521E-04 .26037E-03
18 -.36825E-04 -.21711E-04 .1948NE-04 -.20689E-03 .13545E-03 .42956E-04 -.46107E-03 .58874E-04 .71696E-04 .75573E-04
      -,22325E-03 -,49622E-04 -,11909E-04 .66816E-04 -,12767E-03 .36550E-03 -,15491E-03 .76344E-05 .28254E-03 .23396E-03
      -,51173E-04 -,56617E-04 .48199E-03 -,51173E-04
19 .52471E-04 -.15977E-04 -.16039E-04 -.43244E-04 .12050E-03 -.21959E-03 -.24783E-03 -.89684E-04 .77082E-04 .48321E-04
       .93321E-04 -.13289E-03 .77933E-05 -.79498E-05 .47294E-04 -.10452E-03 -.19987E-03 .28254E-03 .32415E-03 .22615E-03
      -,95164E-04 -,10529E-03 -,22393E-04 -,95164E-04
20 .28167E-04 -.11538E-04 -.86585E-05 -.42251E-04 .78303E-04 -.17505E-03 -.19165E-03 -.71936E-04 .28667E-04 .45702E-04
        .56513E-04 -.11002E-03 -.1592BE-04 -.29016E-04 .46455E-04 -.25164E-03 .94442E-04 .23396E-03 .22615E-03 .66230E-03
        .36870E-03 .40793E-03 .20104E-04 .36870E-03
21 -.22683E-04 .43529E-05 .68991E-05 .22772E-05 -.40351E-04 .45630E-04 .56592E-04 .18252E-04 -.44285E-04 -.3456E-05 .3456E-05 .3456E-05 .3456E-05 .3468E-04 .24085E-04 -.2713F-04 -.2773E-04 -.2775E-05 -.12344E-03 .26037E-03 -.51173E-04 -.95164E-04 .36870E-03
        .40316E-03 .44605E-03 .37384E-04 .40316E-03
22 -.25396E-04 .48159E-05 .76330E-05 .25195E-05 -.44643E-04 .50484E-04 .62613E-04 .20194E-04 -.48996E-04 -.42547E-05
      -.38511E-04 .26647E-04 -.22917E-04 -.19850E-04 -.25198E-05 -.13657E-03 .28807E-03 -.56617E-04 -.18529E-03 .40793E-03
        .44605E-03 .4935UE-03 .41362E-04 .44605E-03
 23 -.83682E-04 -.64459E-05 .33554E-04 -.16108E-03 .21177E-04 .24242E-03 -.22051E-03 .13909E-03 -.95170E-06 .29103E-04 -.30181E-03 .73380E-04 -.18673E-04 .72023E-04 -.16704E-03 .44999E-03 .32521E-04 .48199E-03 -.22393E-04 .20104E-04
         .37384E-04 .41362E-04 .48786E-03 .37384E-04
 24 -.22683E-84 .43529E-85 .68991E-85 .22772E-85 -.48351E-84 .45630E-84 .56592E-84 .18252E-84 -.44285E-84 -.38456E-85
       -,34808E-04 .24085E-04 -,28713E-04 -,17942E-04 -,22775E-05 -,12344E-03 ,26037E-03 -,51173E-04 -,95164E-04 ,36870E-03
         49316E-93 44605E-93 37384E-04 49316E-93
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APPENDIX D (cont)

SUMMARY FOR DIFFERENTIAL PARAMETERS

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XE(1)
                  SX(1)
                              XC(I)
                                           RELXE
                                                      RELXE**2
                                                                   XA(I)
                                                                              SXA(I)
                                                                                            RELXF
                                                                                                      RELXF**2
 1 1.00000E+00 1.00000E-01 1.00000E+00 0.
                                                                9.78M12E+01 1.98243E+02-2.19885E-01 4.83494E+02
 2 1.00000E+00 1.00000E-01 1.00000E+00 0.
                                                   ø.
                                                                9.32236E-01 4.88807E-02-6.77641E-01 4.59197E-01
 3 1.00000E+00 1.00000E+01 1.00000E+00 0.
                                                                9.94606E-01 2.00620E-02-5.39420E-02 2.90974E-03
 4 1.00000E+00 1.00000E-01 1.00000E+00 0.
                                                                9.88789E-01 1.22533E-01-1.12109E-01 1.25684E-02
 5 1.00000E+00 1.50000E-01 1.00000E+00 0.
                                                                9.61475E-01 2.75562E-02-2.56835E-01 6.59644E-02
 6 1.00000E+00 1.00000E-01 1.00000E+00 0.
                                                                9.79102E-01 3.09979E-02-2.08985E-01 4.36747E-02
 7 1.00000E+00 1.50000E-01 1.00000E+00 0.
                                                                8.39995E-01 1.33436E-01-1.06670E+00 1.13785E+00
 8 1.00000E+00 1.00000E-01 1.00000E+00 0.
                                                                1.05883E+00 1.85363E-01 5.88324E-01 3.46125E-01
 9 1.00000E+00 1.00000E=01 1.00000E+00 0.
                                                                1.06331E+00 1.33422E-01 6.33065E-01 4.00771E-01
10 1.00000E+00 1.000UNE-U1 1.00000E+00 A.
                                                                9.79160E+01 1.94011E-01-2.08402E+01 4.34316E-02
11 1.0000AE+0A 1.0000AE+01 1.00AOAE+0A 0.
                                                                1.00134E+00 1.94546E-01 1.34117E-02 1.79872E-04
12 1.00000E+00 1.00000E-01 1.00000E+00 0.
                                                                9.95451E+01 1.94538E+01-4.54924E-02 2.06956E-03
13 1.00000E+00 6.00000E-02 1.00000E+00 0.
                                                                1.13790E+00 1.02834E+01 2.29827E+00 5.28204E+00
14 1.00000E+00 4.00000E-02 1.00000E+00 0.
                                                                1,10604E+00 3,66005E-02 2,65103E+00 7,02798E+00
15 1.PARROE+08 6.RORUGE-02 1.00000E+08 0.
                                                                1.16569E+00 6.94256E-02 2.76147E+00 7.62574E+00
16 1.00000E+00 1.00000E-01 1.00000E+00 0.
                                                   0.
                                                                1.00909E+00 1.94360E-01 9.08541E+02 8.25446E-03
17 1.00000E+00 1.00000E-01 1.00000E+00 0.
                                                   0.
                                                                1.00882E+08 1.93743E-01 8.82264E-02 7.78390E-03
18 1.00000E+00 1.00000E-01 1.00000E+00 0.
                                                                9,95512E+01 1,94528E-01-4,48831E-02 2,01449E-03
19 1.00000E+00 1.00000E-01 1.00000E+00 0.
                                                                1.08546E+00 1.12206E+01 8.54607E+01 7.30352E+01
   ΜJ
                      CHIDI
                                              CHIDE
   19
                                           2.3247E+01
   MK
          CHISI
                                  CHI2F
   43
      5.0282E+02
                               9.0910E+01
```

SUMMARY FOR INTEGRAL PARAMETERS

YE(I) SY(I) YC(1) RELYE RELYE**2 YA(I) SYA(I) RELYF RELYF**2 1 1.00000E+00 4.00000E-03 9.92000E-01-2.00000E+00 4.00000E+00 9.92718E-01 6.68208E-03-1.82041E+00 3.31390E+00 2 1.00000E+00 4.00000E-03 9.92400E-01-1,90000E+00 3.61000E+00 1.00151E+00 5.31330E-03 3.76681E-01 1.41888E-01 3 1.00000E+00 4.00000E-03 9.92700E-01-1.82500E+00 3.33063E+00 1.00187E+00 5.57924E-03 4.66705E-01 2.17813E-01 4 1.00000E+00 2.50000E+02 1.10000E+00 4.00000E+00 1.60000E+01 9.90511E-01 3.53207E-02-3.79562E-01 1.44067E-01 5 1.00000E+00 2.50000E+02 1.15000E+00 6.00000E+00 3.60000E+01 1.01368E+00 3.06338E-02 5.47022E-01 2.99233E-01 6 1.00000E+00 3.50000E-02 1.24000E+00 6.85714E+00 4.70204E+01 1.08997E+00 4.41262E-02 2.57055E+00 6.60774E+00 7 1.00000E+00 7.50000E-02 9.20000E-01-1.06667E+00 1.1377BE+00 8.5337BE-01 4.16583E-02-1.95496E+00 3.821BBE+00 8 1.00000E+00 3.50000E+02 1.25000E+00 7.14286E+00 5.10204E+01 1.05249E+00 3.28765E+02 1.49961E+00 2.24883E+00 9 1.00000E+00 3.50000E-02 1.24000E+00 6.85714E+00 4.70204E+01 1.03574E+00 3.17746E-02 1.02129E+00 1.04284E+00 10 1.00000E+U0 2.50000E-02 1.16000E+00 6.40000E+00 4.09600E+01 9.36055E-01 3.51980E+02-2.55780E+00 6.54233E+00 11 1.00000E+00 3.50000E-02 1.18000E+00 5.14286E+00 2.64490E+01 1.02748E+00 5.25404E-02 7.85003E-01 6.16230E-01 12 1.00000E+U0 3.50000E-U2 1.25000E+00 7.14286E+00 5.1U204E+01 1.04182E+00 3.29078E-02 1.19498E+00 1.42797E+00 13 1. MANUME+UN 3.5000ME-U2 1.2600ME+UN 7.42857E+NN 5.51837E+N1 1.04629E+NN 3.32832E-N2 1.32258E+NN 1.74922E+NN 14 1.00000E+00 3.50000E-02 1.27000E+00 7.71429E+00 5.95102E+01 1.02388E+00 5.27346E-02 6.82303E-01 4.65537E-01 15 1.000000E+00 3.50000E-02 1.09000E+00 2.57143E+00 6.61224E+00 9.59831E-01 5.28047E-02-1.14768E+00 1.31718E+00 16 1.400000E+00 3.40000E-02 9.00000E-01-3.33333E+00 1.11111E+01 9.42179E-01 4.11891E-02-1.92737E+00 3.71474E+00 17 1.00000E+00 3.00000E-02 1.03000E+00 1.00000E+00 1.00000E+00 1.06012E+00 4.20133E+02 2.00387E+00 4.01548E+00 18 1. MDM0ME+00 2. M000ME-02 9. 90M0ME-01-5. M000ME-01 2. 50MMME-01 9. 74651E-01 2. 76305E-02-1. 26746E+0M 1. 60646E+0M 19 1.00000E+00 2.00000E-02 1.05000E+00 2.50000E+00 6.25000E+00 1.03258E+00 1.80042E-02 1.62880E+00 2.65299E+00 20 1.AUN000E+00 2.00000E-02 1.A9000E+00 4.50000E+00 2.02500E+01 1.A5389E+00 2.57353E-02 2.69436E+00 7.25955E+00 21 1.00000E+00 2.00000E+02 9.40000E-01-3.00000E+00 9.00000E+00 9.24455E-01 2.00788E-02-3.77723E+00 1.42675E+01 22 1.000000E+00 2.00000E+02 1.04000E+00 2.00000E+00 4.00000E+00 1.02280E+00 2.22148E-02 1.14009E+00 1.29980E+00 23 1.00000E+00 5.00000E-02 9.60000E-01-8.00000E-01 6.40000E-01 9.61046E-01 2.20075E-02-7.79072E-01 6.06953E-01 24 1.00000E+00 5.00000E-02 9.40000E-01-1.20000E+00 1.44000E+00 9.24455E-01 2.00788E-02-1.51089E+00 2.28279E+00 MK CHIDI CHIDE 24 5.0282E+02 6.7663E+01 MK CHI21 CHI2F 43 5.0282E+02 9.0910E+01

SUMMARY FOR COMBINED PARAMETERS

MK CHIZI CHIDI CHIZF CHIDF DISPR
43 5.0282E+02 5.0282E+02 9.0910E+01 9.0910E+01 3.7879E+00

APPENDIX E

SAMPLE INPUT FOR SENSITIVITY CALCULATION

```
SENSITIVITY ANALYSIS, 41-GP NEUTRON TRANSPORT IN IRON SPHERE
                                                                                                                                                                                                                ALVIN
          2
                                            0
                                                                                                                                                                                                                ALVIN
           1
                           6
                                                                                                                                                                                                                SENSI
DATA FOR SENSITIVITY ANALYSIS CASE ONE OF ONE
                                                                                                                                                                                                                SENSI
                                                                                                                                                                                                                SENSI
                         73
          A
                                                                                                                                                                                                                SENST
  .0848 E+00
                                                                                                                                                                                                                SENSI
                         74
                                          41
                                                              ø
                                                                            17
                                                                                               6
                                                                                                                                                                                                              REDFLX
           6
                                                                                                                                                                                                              CROSEC
8.01443E-09
                                                                                                APPENDIX F
                                                              SAMPLE OUTPUT FOR SENSITIVITY CALCULATION
           SENSITIVITY ANALYSIS, 41-GP NEUTRON TRANSPORT IN JHON SPHERE
                          KSENS
                                                   KADJST
                                                                                MI
                                                                                                         LM
                                                                                                            0
            DATA FOR SENSITIVITY ANALYSIS CASE ONE OF ONE
                                                                              KGEOM
                                                      NXR
                                                                                                                                NSAVE
                             NYR
                                                                                                          NR
                                                                                                                                                         KTIMS
                                                                                                                                                                                        ΝT
                                                                                                                                                                                                       KTYPE
                                                                                   5
                                                                                                                                     Ø
                                                                                                                                                               0
                                        IMMIN(IR), IMMAX(IR), IR=1, NR
                                        DENS(IR), IR=1, NR
            .848000E-01
                       KFLUX
                                                    NM
                                                                             NG
                                                                                                      NLR
                                                                                                                                NA
                                                                                                                                                         NL
                                                                                                                                   17
                                                      74
                                                                                41
                                      (RM(IM), IM=1, NM+1)
            INPUT RADII(J), J=1,75
                                              .250000E+01 .500000E+00 .750000E+00 .100000E+01 .200000F+01
            .300000E+01 .400000E+01 .500000E+01 .700000E+01 .700000E+01 .800000F+01 .800000F+01 .900000E+01 .100000E+01 .100000E+01 .100000E+02 .120000E+02 .130000E+02 .140000F+02 .150000E+02 .160000E+02 .170000E+02 .180000E+02 .190000E+02 .260000F+02 .260000E+02 .270000E+02 .270000E+02 .270000E+02 .270000E+02 .370000E+02 .37000E+02 .3700E+02 .3700E+02 .3700E+02 .3700E+02 .
            (QCOSA(TA), TA=1, NA)
          COSINE(I), J=1,17)
          -.10M0MUE+01-.982031E+0U-.91M582E+0M-.833W27E+WW-.747468E+MW-.65W756E+MM
          -.536897E+00-.391194E+00-.133446E+00 .133446E+00 .391194E+00 .536897F+00 .650756E+00 .747468F+00 .833027E+00 .910582E+00 .982031E+00
                                         (QWTSA(IA), IA=1, NA)
          WEIGHT(I), J=1,17
            .523245E-01 .454261F-01 .402441F-01 .367965F-01 .270771E-01
```

R

APPENDIX F (cont)

```
(RM(IM), IM=1, NM+1)
 INPUT RADII(J), J=1,75
Ø.
 .570000E+02 .580000E+02 .590000E+02 .610000E+02 .610000E+02 .50000E+02
 .630000E+02 .640000E+02 .650000E+02 .660000E+02 .670000F+02 .680000F+02 .690000F+02 .700000E+02 .710000F+02
              (QCOSA(IA), TA=1, NA)
COSINE(I), I=1,17)
 COSINES MULT BY -1. IN REDFLX FOR ADJOINT FLUX EXPANSION
 .100000E+01 .982031E+00 .910582E+00 .833027E+00 .747468E+00 .650756F+00 .536897E+00 .391194E+00 .133446E+00-.133446E+00-.391194E+00-.536897F+00
-.650756E+00-.74746BE+00-.833027E+00-.910582E+00-.982031F+00
              (QWTSA(IA), IA=1, NA)
WEIGHT(I), 1=1,17
 .270771E-01 ,367965E-01 .402441E-01 .454261E-01 .523245E-01 .628440E-01 .907613E-01 ,144526E+00 ,144526E+00 .907613E-01 .628440F-01 .523245E-01 .454261E-01 .402441E-01 .367965E-01 .270771E-01
         NLCX
                                                                    AFTER CHANGE IN CRANGE
AFTER CHANGE IN CRANGE
 PR FE OF PU-PB, 41GP CROSS SECTIONS ADJ TO EXP VAL
 P1 FE OF P0-P8,41GP CROSS SECTIONS ADJ TO EXP VAL
 P2 FE OF P8-P8,41GP CROSS SECTIONS ADJ TO EXP VAL
                                                                    AFTER CHANGE IN CRANGE
                                                                    AFTER CHANGE IN CRANGE
AFTER CHANGE IN CRANGE
 P3 FL UF P0-P8,41GP CROSS SECTIONS ADJ TO EXP VAL
 P4 FE OF P0-P8,41GP CROSS SECTIONS ADJ TO EXP VAL
P5 FE OF P0-P8,41GP CROSS SECTIONS ADJ TO EXP VAL
                                                                    AFTER CHANGE IN CRANGE
 .801443E-08
```

APPENDIX F (cont)

SENSITIVITY PROFILE

GROUP	SENSITIVITY
1	0.
5	0.
3	0.
4	0.
5	0.
6	0.
7	0.
8 9	+1.52696E=04
10	-1.02585E-02
11	-7.16549E-03 -4.26670E-03
12	-1.75711E-03
13	-1.83075E-03
14	-1.10495E-03
15	-1.15348E-03
16	-1.15511E-03
17	-9.72420E-04
18	-2.16578E-03
19	-1.46277E-03
201	-2.03188E-03
21	-2.80632E-03
2 2	-3.94025E-03
23	-9.26679E-03
24	-3.24802E-02
25	-5.23364E-02
26	-9.26052E-03
27 ·	-2.59525E-02
28	-3,21015E-03
29	-1.99605F-03
30	-4.84289E-04
31 32	-3.99885E-04 -1.83508E-04
32 33	-1.68276E-04
33 34	-1.53271E-04
35	-1.35074E-04
36	-1.06397E-04
37	-7.35754E-05
38	-4.06675E-05
39	-1.55001E-05
40	-4.99287E-06
41	-1.19203E-06