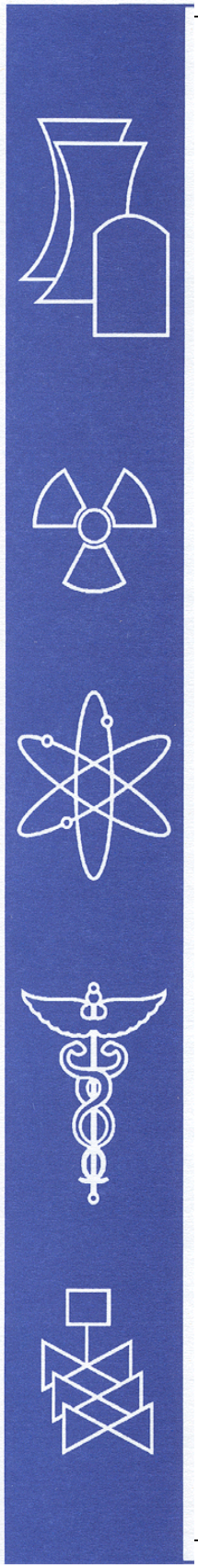
NUREG/CR-5719
ORNL/TM-13738



SEN1: A One-Dimensional Cross-Section Sensitivity and Uncertainty Module for Criticality Safety Analysis

Prepared by
R. L. Childs

Oak Ridge National Laboratory

U.S. Nuclear Regulatory Commission
Office of Nuclear Regulatory Research
Washington, DC 20555-0001

AVAILABILITY NOTICE

Availability of Reference Materials Cited in NRC Publications

NRC publications in the NUREG series, NRC regulations, and Title 10, Energy, of the Code of Federal Regulations, may be purchased from one of the following sources:

1. The Superintendent of Documents
   U.S. Government Printing Office
   PO. Box 37082
   Washington, DC 20402-9328
   <http://www.access.gpo.gov/su_docs>
   202-512-1800

2. The National Technical Information Service
   Springfield, VA 22161-0002
   <http://www.ntis.gov/ordernow>
   703-487-4650

The NUREG series comprises (1) brochures (NUREG/BR-XXXX), (2) proceedings of conferences (NUREG/CP-XXXX), (3) reports resulting from international agreements (NUREG/IA-XXXX), (4) technical and administrative reports and books [(NUREG-XXXX) or (NUREG/CR-XXXX], and (5) compilations of legal decisions and orders of the Commission and Atomic and Safety Licensing Boards and of Office Directors' decisions under Section 2.206 of NRC's regulations (NUREG-XXXX).

A single copy of each NRC draft report is available free, to the extent of supply, upon written request as follows:

Address: Office of the Chief Information Officer
Reproduction and Distribution
Services Section
U.S. Nuclear Regulatory Commission
Washington, DC 20555-0001

E-mail: <DISTRIBUTION@nrc.gov>
Facsimile: 301-415-2289

A portion of NRC regulatory and technical inforrnation is available at NRC's World Wide Web site:

<http://www.nrc.gov>

All NRC documents released to the public are available for inspection or copying for a fee, in paper, microfiche, or, in some cases, diskette, from the Public Document Room (PDR):

NRC Public Document Room
2120 L Street, N.W., Lower Level
Washington, DC 20555-0001
<http://www.nrc.gov/NRC/PDR/pdr1.htm>
1-800-397-4209 or locally 202-634-3273

Microfiche of most NRC documents made publicly available since January 1981 may be found in the Local Public Document Rooms (LPDRS) located inthe vicinity of nuclear power plants. The locations of the LPDRs may be obtained from the PDR (see previous paragraph) or through:

<http://www.nrc.gov/NRC/NUREGS/SR1350/V9/lpdr/html>

Publicly released documents include, to name a few, NUREG-series reports; Federal Register notices; applicant, licensee, and vendor documents and correspondence; NRC correspondence and internal memoranda; bulletins and information notices; inspection and investigation reports; licensee event reports; and Commission papers and their attachments.

Documents available from public and special technical libraries include all open literature items, such as books, journal articles, and transactions, Federal Register notices, Federal and State legislation, and congressional reports. Such documents as theses, dissertations, foreign reports and translations, and non-NRC conference proceedings may be purchased from their sponsoring organization.

Copies of industry codes and standards used in a substantive manner in the NRC regulatory process are maintained at the NRC Library, Two White Flint North, 11545 Rockville Pike, Rockville, MD 20852-2738. These standards are available in the library for reference use by the public. Codes and standards are usually copyrighted and may be purchased from the originating organization or, if they are American National Standards, from—

American National Standards Institute
11 West 42nd Street
New York, NY 10036-8002
<http://www.ansi.org>
212-642-4900

NUREG/CR–5719
ORNL/TM–13738

SEN1: A One-Dimensional Cross-Section Sensitivity and Uncertainty Module for Criticality Safety Analysis

Manuscript Completed: June 1999
Date Published: July 1999

Prepared by
R. L. Childs

Oak Ridge National Laboratory
Managed by Lockheed Martin Energy Research Corporation
Oak Ridge, TN 37831–6370

C. W. Nilsen, NRC Project Manager

Prepared for
Division of Systems Analysis and Regulatory Effectiveness
Office of Nuclear Regulatory Research
U.S. Nuclear Regulatory Commission
Washington, DC 20555–0001
NRC Job Code W6479

ABSTRACT

This report documents sensitivity analysis computer codes that have been developed for use with one-dimensional (1-D) and two-dimensional (2-D) calculational models. These codes provide a useful tool to aid criticality safety analysts in understanding the applicability of selected critical experiments to the validation of real systems.

SEN1 is a prototypic SCALE control module that facilitates the application of sensitivity theory to criticality safety analysis. The XSDRNPM module uses the method of discrete ordinates to calculate k_{eff} for applications that are appropriate for 1-D modeling. Perturbation theory is used to determine the sensitivity of the calculated value of k_{eff} to the nuclear data used in the calculation as a function of nuclide, reaction type, and energy. The uncertainty in the calculated value of k_{eff}, resulting from uncertainties in the basic nuclear data used in the calculation, is estimated using energy-dependent relative covariance matrices processed from ENDF/B-V. Systems containing arrays of fuel pins may be analyzed using cell-weighted cross sections. The methods used in this work are based on the FORSS system developed at ORNL in the 1970s. The present work uses the XSDRNPM module and the problem- dependent cross-section processing capabilities of the SCALE system and is much more automated than the earlier FORSS system. Two-dimensional sensitivity analysis using the DORT code has also been developed and is described in the appendix.

CONTENTS

CONTENTS (continued)

LIST OF FIGURES

LIST OF TABLES

ACKNOWLEDGMENTS

This work was supported by the Nuclear Regulatory Commission (NRC) under Project JCN W6479, Development and Applicability of Criticality Safety Software for Licensing Review. The direction of C. W. Nilsen, the NRC project manager, along with S. A. Parra and K. J. Hardin, the NRC technical monitors, is acknowledged.

The careful review of the manuscript by B. L. Broadhead, S. M. Bowman, L. M. Petrie, C. V. Parks, and B. T. Rearden is much appreciated. L. M. Petrie provided valuable guidance concerning the development of SCALE control sequences.

1 INTRODUCTION

SCALE[1] is a modular code system for performing standardized computer analyses for licensing evaluation that was developed at Oak Ridge National Laboratory for the U.S. Nuclear Regulatory Commission. SEN1 is a prototypic SCALE control module that facilitates the application of sensitivity theory to criticality safety analysis. The module prepares sensitivity coefficients that relate the changes in the system multiplication factor with changes in the underlying nuclear data. Plans call for the inclusion of a production version of SEN1 in version 5.0 of SCALE. SEN1 provides automated, problem-dependent cross sections using the same methods and input as the Criticality Safety Analysis Sequences (CSAS) in SCALE. The SEN1 sequence calls the cross-section processing codes BONAMI and NITAWL just as the CSAS control sequences do. The SEN1X sequence calls BONAMI, NITAWL, and XSDRNPM to provide cell-weighted cross sections similar to the CSAS1X sequence. After the cross sections are processed, SEN1 (or SEN1X) calls two XSDRNPM criticality calculations, one forward and one adjoint. Finally, SEN1 calls the codes VIP1D and LAKE. VIP1D reads forward and adjoint flux files written by XSDRNPM and writes an interface file used by LAKE. LAKE calculates sensitivity coefficients that indicate the sensitivity of the calculated value of k_{eff} to changes in the cross sections and the uncertainty in the calculated value of k_{eff} due to uncertainties in the basic nuclear data.

Formats and procedures were adopted for the Evaluated Nuclear Data Files (ENDF/B) that allowed the evaluators to represent the estimated uncertainties in the basic nuclear data. These covariance files contain the uncertainties and the correlations in the data for a number of isotopes that are important for criticality safety analyses. Multigroup covariance matrices processed from the ENDF/B data are used with multigroup sensitivity coefficients to calculate the uncertainty in k_{eff} resulting from the uncertainties in the nuclear data. The uncertainty in calculated values of k_{eff} for critical experiments analyzed to date with SEN1 and ENDF/B-V data have varied from 0.8 to 2.4%. These uncertainty estimates give the criticality safety analyst additional information about the calculated system that is not provided by the computer codes commonly used for criticality safety analysis.

In addition to their use in uncertainty analysis, multigroup sensitivity coefficients provide information about the importance of cross sections to the calculated value of k_{eff} as a function of isotope, reaction type, and energy. This information allows the analyst to compare different systems, such as a critical experiment and a proposed application, based on which nuclear data are important contributors to the calculated k_{eff} for each system.

The FORSS[2,3] computer code system for sensitivity and uncertainty analysis was developed in the 1970s at Oak Ridge National Laboratory over about a five-year period. The methods used for sensitivity and uncertainty analysis in the present work are based on the work done for FORSS. The XSDRNPM module of SCALE is used to calculate forward and adjoint fluxes; the FORSS system used the ANISN code. The equations used to calculate the sensitivity coefficients are the same as those used in the JULIET module of FORSS, but the equations were reprogrammed to provide a more readable and maintainable code for future development. The uncertainty analysis in LAKE uses the formulation developed for the CAVALIER module of FORSS. Two interface file formats developed for the FORSS system are used to store information. These formats are used in the SENPRO file for storing sensitivity coefficients and in the COVERX interface file for storing cross-section covariance data.

A COVERX covariance file containing 23 nuclides has been produced in the SCALE 44-group library group structure using ENDF/B-V covariance data. The PUFF-2 computer code, originally developed for the FORSS system, was used to process the data. SEN1 is written to use any valid COVERX covariance file. This flexibility allows the covariance file to be updated or replaced with no code modifications. The fact that the covariance files are in 44 groups does not mean that the sensitivity analysis must use the 44-group library.

Other ENDF/B-V libraries, such as the SCALE 238-group library, may be used. The system models are allowed to contain nuclides other than the ones found on the covariance files. However, the uncertainties in these nuclides will be assumed to be zero for purposes of calculating the uncertainty in k_{eff} due to nuclear data. The calculated uncertainty will be a lower bound in these cases.

In addition to the SENPRO interface file, LAKE also writes the sensitivity coefficients in a formatted file. This file is used to produce plots of sensitivity coefficients. Plotting is not done by the SEN1 sequence, but plotting codes have been developed for IBM UNIX workstations and Windows 95/98/NT personal computers.

Appendix A describes two-dimensional (2-D) sensitivity/uncertainty analysis using the DORT[4] code. Conceptually, the 2-D procedures are similar to the one-dimensional (1-D) procedures, with DORT transport calculations replacing the XSDRNPM transport calculations.

2 SENSITIVITY ANALYSIS

Sensitivity coefficients are calculated using perturbation theory. In operator notation, the forward form of the neutron transport equation may be written as

$$A\phi = \frac{1}{k} B\phi \ , \qquad \textbf{(2.1)}$$

where

k = k_{eff}, the neutron multiplication factor,

A = an operator that represents all of the transport equation, except for the fission term,

B = an operator that represents the fission term in the transport equation.

In addition to the forward transport equation, the XSDRNPM module of SCALE also solves the adjoint form of the neutron transport equation to obtain the multigroup adjoint flux, ϕ^*. The adjoint flux is an importance function that gives the relative importance to k_{eff} of neutrons at different spatial intervals and energy groups.

Using linear perturbation theory, one can show that the relative change in k due to a perturbation of the transport operator is given to first order (valid for small perturbations) by

where < > represents an integration over all phase space. The integration is over all space intervals, all energy groups, and all angular space, as represented by the angular quadrature. δA and δB represent the changes in the transport operator.

This perturbation equation can be applied to a wide variety of perturbations (such as changing the angular distribution of inelastic scattering). Consider the special case of perturbing the number density of a single nuclide in a single zone. Any size change may be considered, because the result varies linearly with the perturbation. If the number density of a nuclide is doubled, then the change in the transport operator is simply the portion of the transport operator corresponding to the nuclide.

Since first-order perturbation theory approaches the exact result in the limit as the size of the perturbation approaches zero, the correct mathematical interpretation of the number density perturbation described above is as a derivative,

$$S_N = \frac{N}{k} \frac{dk}{dN} \ . \qquad \textbf{(2.3)}$$

Physically, this sensitivity coefficient is an estimate of the contribution of the nuclide in question to the value of k_{eff}. For example, if the sensitivity coefficient for changing the number density of ^{234}U in an XSDRNPM criticality calculation is -0.001, then repeating the XSDRNPM calculation with the ^{234}U number density set to

zero would result in a calculated k_{eff} that is approximately 0.001 higher than the original calculated value. If the number density sensitivity coefficient for ^{235}U is 0.7, then increasing the ^{235}U number density by 1% would result in an increase in the calculated value of k_{eff}, which would be approximately 0.7%. The reason these predicted changes are approximate is that k_{eff} does not vary linearly with number density change, and thus the predictions are only appropriate for small perturbations. It is difficult to quantify what constitutes a small perturbation.

The number density sensitivity coefficient can also be interpreted as changing all of the cross sections of the isotope the same proportional amount. In terms of mathematics, this can be viewed as applying an energy-independent multiplicative scale factor to all energy groups and reactions. The sensitivity coefficient or relative sensitivity of k_{eff} for changes in the total cross section as a function of energy group is defined as

$$S_{g,total} = \frac{\sigma_{g,total}}{k} \frac{dk}{d\sigma_{g,total}} . \quad \textbf{(2.4)}$$

$S_{g,total}$ and S_N are both evaluated using Eq. (2.2). The only difference is that a sensitivity coefficient is calculated for each energy group, g. The energy integrated sensitivity coefficient is defined by

$$S_{total} = \sum_g S_{g,total} . \quad \textbf{(2.5)}$$

Also note that

$$S_{total} = S_N . \quad \textbf{(2.6)}$$

The sensitivity coefficients for other nuclear reactions can also be evaluated. Consider the following definition:

$$\sigma_{total} = \sigma_{capture} + \sigma_{scatter} + \sigma_{fission} . \quad \textbf{(2.7)}$$

The capture cross section is neutron disappearance (MT 101 using ENDF conventions), not just radiative capture (MT 102). The fission cross section is MT 18. The scattering cross section in Eq. (2.7) includes elastic scattering (MT 2), inelastic scattering, and all other reactions such as (n,2n), where neutrons emerge from the collision. The sensitivity coefficients for the three nuclear reactions in Eq. (2.7) are calculated using Eq. (2.2), as is the total sensitivity coefficient. The relationship between these sensitivities is

$$S_{g,total} = S_{g,capture} + S_{g,scatter} + S_{g,fission} . \quad \textbf{(2.8)}$$

3 SENSITIVITY COEFFICIENT GENERATION

In this section, the equations used in the LAKE code called by the SEN1 control sequence to calculate sensitivity coefficients are given. These equations are programmed in the LAKE code called by the SEN1 control sequence. In order to emphasize the most important aspects of these definitions, the equations are given for a single nuclide and a single mesh cell (spatial interval). To obtain sensitivity coefficients for a zone, the sensitivity coefficients for all of the mesh cells in the zone are summed.

Energy-integrated sensitivities are obtained by summing the group-dependent sensitivity coefficients. Energy-integrated sensitivities are denoted by dropping the group subscript.

3.1 SENSITIVITY COEFFICIENTS FOR AVERAGE NEUTRONS PER FISSION NU-BAR ($\bar{\nu}$)

Consider a single mesh cell and one of the fissionable isotopes in that mesh cell. The sensitivity coefficient for changing $\bar{\nu}$ in this mesh cell is

$$S_{g,\bar{\nu}} = \frac{VN\bar{\nu}_g\sigma_f^g\phi_g(\sum_{g'}\phi_{g'}^*\chi_{g'})}{D} , \qquad \textbf{(3.1)}$$

where

- V = the volume of the mesh cell,
- N = the number density of the nuclide in the interval,
- $\bar{\nu}_g$ = the average number of neutrons per fission for the nuclide in group g,
- σ_f^g = the group g fission cross section for the nuclide in the mesh cell,
- ϕ_g = the group g flux in the mesh cell,
- ϕ_g^* = the adjoint group g flux in the mesh cell,
- χ_g = the fission spectrum for the nuclide in group g,
- D = the denominator of Eq. (2.2) (defined below).

The sensitivity coefficient for a zone is obtained by summing the sensitivity coefficients for all of the mesh cells in the zone.

The energy-integrated sensitivity is obtained by summing over all energy groups. Thus,

$$S_{\bar{\nu}} = \sum_g S_{g,\bar{\nu}} . \qquad \textbf{(3.2)}$$

The value of D is given by

$$D = \sum_{\substack{\text{nuclides,}\\ \text{intervals}}} V\left(\sum_g N \bar{\nu}_g \sigma_f^g \phi_g\right)\left(\sum_{g'} \phi_{g'}^* \chi_{g'}\right) , \qquad \textbf{(3.3)}$$

where the summation is over all space intervals and fissionable nuclides. Subscripts for the space interval and nuclide are omitted. The two terms in parentheses may be considered forward and adjoint fission densities for the nuclide.

Notice that the sum of all $S_{\bar{\nu}}$ for a problem is 1.0. This means that artificially multiplying $\bar{\nu}$ for all nuclides and energies by any constant causes the calculated value of k_{eff} to increase by that same constant multiplier.

XSDRNPM does not use the fission spectrum of each different isotope in a mixture but instead uses a single fission spectrum for each mixture that is a weighed average of the fission spectra for the nuclides in the mixture. This difference raises the question of which fission spectrum to use for the calculation of sensitivity coefficients. Presently, the individual nuclide fission spectrum is used to calculate the numerator of Eq. (3.1), but the average fission spectra are used to calculate D. This method causes the summation of all of the $\bar{\nu}$ sensitivities to deviate from unity, and the magnitude of the deviation is an estimate of the effect of using the averaged fission spectra. For all systems considered so far, this effect has been insignificant.

The MT number for $\bar{\nu}$ is 452. MT numbers are used in both the SENPRO and COVERX interface files to identify reaction types.

3.2 SENSITIVITY COEFFICIENTS FOR FISSION SPECTRUM CHI (χ)

Sensitivity coefficients for χ are closely related to $\bar{\nu}$ sensitivity coefficients and can be used to estimate the effect of changing the fission spectrum. The equation for the χ sensitivity coefficient for one space mesh and nuclide is

$$S_{g,\chi} = \frac{V \chi_g \phi_g^* \left(\sum_{g'} N \bar{\nu}_{g'} \sigma_f^{g'} \phi_{g'}\right)}{D} . \qquad \textbf{(3.4)}$$

Note the similarity between Eqs. (3.1) and (3.4). Also, note that

$$S_\chi = S_{\bar{\nu}} . \qquad \textbf{(3.5)}$$

This effect can be seen in the printout of the sensitivity sequence and in the plots of sensitivity profiles. Even though the energy dependence of the $\bar{\nu}$ and χ sensitivity coefficients differ, the energy-integrated values are identical.

The MT number for χ is 1018.

3.3 CAPTURE CROSS-SECTION SENSITIVITY COEFFICIENTS

The sensitivity coefficient for any reaction *x* that causes neutron disappearance in a single mesh cell is

$$S_{g,x} = \frac{-k}{D} N \sigma_x^g T_g \ , \qquad \textbf{(3.6)}$$

where

$$T_g = V \sum_m \phi_{g,m} \phi^*_{g,m} W_m \ , \qquad \textbf{(3.7)}$$

and

$\phi_{g,m}$ = the forward angular flux in direction m and group g,
$\phi^*_{g,m}$ = the adjoint angular flux in direction m and group g,
W_m = the quadrature weight for direction m.

As before, sensitivity coefficients for a zone are obtained by summing the sensitivity coefficients for each interval over all intervals in the zone.

Sensitivity coefficients are calculated for the following MT numbers:

MT	Reaction
101	Neutron disappearance
102	n,γ
103	n,p
104	n,d
105	n,t
106	n,^{3}He
107	n,α

MT 101 is the sum of all MT reactions from MT 102 to MT 114. In the output of the LAKE code, the sensitivity for MT 101 is called "capture." The sensitivity for MT 101 is used to calculate the sensitivity coefficient for the total cross section.

3.4 FISSION CROSS-SECTION SENSITIVITY COEFFICIENTS

Increasing the fission cross section has (1) a positive effect that results from the change in the fission's source and (2) a negative effect that results from the increase in the total cross section. In the fission source, increasing the fission cross section has the same effect as increasing $\bar{\nu}$ since they appear as a product. However, increasing the fission cross section increases neutron absorption, while increasing $\bar{\nu}$ does not. The fission sensitivity coefficient for one space cell and nuclide is given by

$$S_{g,\text{fission}} = S_{g,\bar{\nu}} - \frac{k}{D} N \sigma_f^g T_g \ . \quad \textbf{(3.8)}$$

Note that the fission sensitivity coefficient is always less than the $\bar{\nu}$ sensitivity coefficient. Because the sum of all $\bar{\nu}$ sensitivity coefficients for a system is 1.0, the sum of all fission sensitivity coefficients is less than 1.0. The fission sensitivity coefficient is used to calculate the total cross-section sensitivity coefficient.

The MT number for fission is 18.

3.5 SCATTERING CROSS-SECTION SENSITIVITY COEFFICIENTS

For a single nuclide and space mesh cell, the sensitivity coefficient for scattering is

$$S_{g,\text{scatter}} = \frac{k}{D} [(\sum_{\ell=0}^{\text{ISCT}} \sum_{g'} N \sigma_{s,g\rightarrow g'}^{\ell} P_{g,g'}^{\ell}) - N \sigma_s^g T_g] \ , \quad \textbf{(3.9)}$$

where

σ_s^g = the scattering cross section for group g and is calculated by subtracting capture and fission from the total cross section,

$\sigma_{s,g\rightarrow g'}^{\ell}$ = the cross section for scattering from group g to g'.

The ℓ superscript indicates that the angular dependence of the scattering cross section is represented by a Legendre series.

For slab and spherical geometry,

$$P_{g,g'}^{\ell} = V \phi_{g,\ell} \phi_{g',\ell}^{*} \ . \quad \textbf{(3.10)}$$

The ℓ subscript indicates that the angular dependence of the angular forward and adjoint fluxes have been expanded in Legendre series.

For cylindrical geometry,

$$P_{g,g'}^{\ell} = V \sum_{n} \phi_{g,\ell,n} \phi_{g',\ell,n}^{*} \ . \quad \textbf{(3.11)}$$

The ℓ and n subscripts indicate that the angular dependence of the forward and adjoint fluxes are represented by spherical harmonic expansions.

Eq. (3.9) is used to evaluate the sensitivity coefficients for all scattering, which includes elastic scattering, inelastic scattering, and (n,2n). This combined scattering sensitivity coefficient is used in the calculation of the total cross-section sensitivity coefficients. Because there is no ENDF MT number for combined scattering, an MT of 0 is used on the SENPRO interface file.

Eq. (3.9) can also be used for other scattering reactions. For example, if the 1-D elastic-scattering cross section is used for σ_s^g and the 2-D elastic scattering matrix is used for $\sigma_{s,g\to g'}^{\ell}$, then the elastic-scattering cross-section sensitivity coefficients are obtained. Sensitivity coefficients are calculated for the following reactions:

MT	Reaction
2	Elastic scattering
4	Inelastic scattering
16	n,2n

3.6 TOTAL CROSS-SECTION SENSITIVITY COEFFICIENTS

Total cross-section sensitivity coefficients are calculated by summing the sensitivity coefficients for capture, scattering, and fission, as indicated in Eq. (2.8). The MT number for the total cross section is 1.

3.7 SUMMARY OF SENSITIVITY COEFFICIENTS CALCULATED

Sensitivity coefficients are calculated and stored on a SENPRO interface file for the following reactions:

MT	Reaction
1	Total
2	Elastic scattering
4	Inelastic scattering
16	n,2n
18	Fission
101	Neutron disappearance
102	n,γ
103	n,p
104	n,d
105	n,t
106	n,^{3}He
107	n,α
452	$\bar{\nu}$
1018	χ

In addition to these reactions, the sensitivity of all scattering reactions is calculated and arbitrarily assigned an MT of 0.

4 UNCERTAINTY ANALYSIS

In the FORSS sensitivity and uncertainty system, the CAVALIER computer program was developed to compute the relative standard deviations of performance parameters (such as k_{eff}), resulting from uncertainties in the basic nuclear data. A rewritten version of CAVALIER is used as a subroutine (CAVA) called by the LAKE code in the SEN1 sensitivity sequence. The original CAVALIER required the user to input a list of the nuclear data (isotope and MT number) to be included in the uncertainty calculation while the rewritten version automatically compiles a list of all nuclear data for which sensitivity profiles and covariance matrices are available. The uncertainty calculation is unchanged; a brief description follows.

The uncertainties in basic nuclear data are described by multigroup relative covariance matrices. An element in a relative covariance matrix is defined by

$$\mathrm{Cov}\,(x_g, y_{g'}) = \frac{\langle x_g - \bar{x}_g \rangle \langle y_{g'} - \bar{y}_{g'} \rangle}{\bar{x}_g \, \bar{y}_g} \quad . \tag{4.1}$$

This equation is the covariance of reaction X (isotope and MT number), group g, and reaction Y, group g'. X and Y can be the same or different. The bar indicates average value, and the angle brackets represent expectation value.

The standard deviation (σ) for the calculated value of k_{eff} due to nuclear data uncertainties is given by the following equation:

$$\sigma^2 = \sum_{\substack{x,y,\\ g,g'}} S_{g,x} \; \mathrm{Cov}(x_g, y_{g'}) \, S_{g',y} \quad . \tag{4.2}$$

The sensitivity coefficients in this equation are described in the previous section. If a nuclide appears in more than one zone, the zonewise sensitivities are summed to obtain system sensitivity coefficients. This summation can give rise to an inaccuracy because resonance-shielded cross sections that vary by zone are used to calculate the zonewise sensitivity coefficients; the cross-section covariance files are for infinite-dilute cross sections. This treatment assumes that the relative uncertainties of shielded cross sections are similar to the relative uncertainties of unshielded cross sections.

A covariance file containing relative covariance matrices for the 23 nuclides listed in Table 4.1 has been processed in the SCALE 44-energy-group structure using the PUFF-2 computer code developed for the FORSS project and ENDF/B-V data. The CAVALIER code allows the group structure of the sensitivity coefficients to be different than the group structure of the covariance matrices. In this case, the sensitivity coefficients are converted to the group structure from the COVERX covariance file. Isotopes are identified using the ZA number, rather than ENDF MAT numbers.

Table 4.1 Nuclides on the ENDF/B-V COVERX covariance file

Nuclide	ID
H	1001
^{10}B	5010
C	6012
N	7014
O	8016
F	9019
Na	11023
Al	13027
Si	14000
Mn	25055
Fe	26000
Cr	27000
Ni	28000
Pb	82000
^{232}Th	90232
^{235}U	92235
^{238}U	92238
^{237}Np	93237
^{239}Pu	94239
^{240}Pu	94240
^{241}Pu	94241
^{242}Pu	94242
^{241}Am	95241

5 SEN1 PROGRAM DESCRIPTION

The SEN1 control module was developed by modifying the existing SCALE control module SAS1. This approach had the advantage that the cross-section processing part of SAS1 could be used unchanged. The main change is to replace the part of SAS1 that performs an XSDRNPM shielding calculation, followed by a XSDOSE calculation. The functions performed by SEN1 are the following:

1. Process cross sections (same as SAS1 or CSAS).

2. Perform a forward XSDRNPM criticality calculation.

3. Perform an adjoint XSDRNPM criticality calculation.

4. Perform a sensitivity and uncertainty analysis using the codes VIP1D and LAKE. These codes are described in the next two sections.

The subroutines used by SEN1 are very similar to those used by SAS1. The following seven subroutines from SAS1 having to do with sources and dose are not used in SEN1:

SOURCE
DOSD1
DOSD2
CORMIX
SNORM
XSDOSA
BFLUX

Three of the subroutines from SAS1 required very minor changes:

RDZON - This subroutine reads the zone description data. In SAS1 the source identifier ISZ is read. RDZON was modified not to read ISZ.

RDICE - This subroutine reads the mixing table data in SAS1. It was modified to also read the problem title. This step was done so that only one title is entered for the problem. The first 16 characters of the title are used on plots and on the SENPRO interface file.

SETB - SETB reads optional parameter values that override the default values. The default values for ICM, XNF, EPS, and PTC are different in SEN1 than in SAS1.

Four of the subroutines from SAS1 were heavily modified:

SAS1 - The name of the subroutine is changed to SEN1. SEN1 communicates with the SCALE driver. Changes were made to perform the functions described earlier in this section.

DATIN - DATIN calls all the subroutines used for data input and data processing needed to prepare the XSDRNPM input data file. The principal changes in this routine were to remove calls to the subroutines listed above that are not needed for a criticality calculation.

SETA - SETA reads the coordinate system specification and boundary conditions. It was modified to allow the right boundary condition to be specified. The specifications for this input were changed to be more like the corresponding input for the Material Information Processor (MIP).

XSDRNA - This subroutine prepares the input data required by XSDRNPM. XSDRNA was modified to prepare data for a criticality case, rather than a shielding case.

One new subroutine was added to SEN1 that was not in SAS1:

ADJOINT - This subroutine is called by SEN1. It reads the XSDRNPM input file written on unit 98 and rewrites the file with the adjoint input parameter ITH set to 1 and the sensitivity output unit NTD set to 32. NTD is set to 31 for the forward case.

6 VIP1D PROGRAM DESCRIPTION

VIP1D is a computer program that reads the output files written by forward and adjoint XSDRNPM cases and writes a file to be read by the LAKE program. As described in Sect. 3, certain quantities involving the product of forward and adjoint fluxes (or flux moments) are required to calculate sensitivity coefficients. These products are seen in Eqs. (3.7), (3.10), and (3.11). These flux products integrated over the volume of a zone are all the flux or adjoint flux information required to calculate sensitivity coefficients for a zone. VIP1D calculates these volume-integrated products and writes them on a file for use by LAKE. Other transport codes, such as DORT, can also be used to calculate forward and adjoint fluxes. Another code, VIP2D, has been developed to process DORT fluxes and write the interface file used by LAKE. This approach allows the same version of LAKE to be used with both XSDRNPM and DORT. VIP2D is described in Appendix A.

The calculations performed by VIP1D use only fluxes and volumes. In particular, a cross-section file is not required, which allows VIP1D to be fairly short and easy to maintain.

As part of the development of the SEN1 control sequence, the XSDRNPM module of SCALE was modified to allow the writing of a new interface file containing information needed for sensitivity calculations. This information is written on unit NTD when NTD is positive. In the SEN1 control sequence, NTD is 31 for the forward case and 32 for the adjoint case. The files written are ft31f001 and ft32f001, respectively.

6.1 XSDRNPM FORWARD OUTPUT FILE

For a forward case, XSDRNPM writes the following unformatted records on unit NTD:

RECORD 1: IZM,IM,MXX,MS,ISCT,MM,JT,IGM

IZM	Number of zones
IM	Number of spatial intervals
MXX	Number of compositions (mixtures)
MS	Length of the XSDRNPM mixing table
ISCT	Order of the Legendre scattering expansion
MM	Number of angles in the angular quadrature
JT	Number of flux moments
IGM	Number of energy groups

RECORD 2: IGE,IBL,IBR,ISN,IFTG,MMT,NT1,T

IGE	Geometry: 1/2/3 = plane/cylinder/sphere
IBL	Left-boundary condition: 0/1/2/3 = vacuum/reflected/periodic/white
IBR	Right-boundary condition
ISN	S_n quadrature order
IFTG	First thermal group

MMT	Number of neutron groups
NT1	Unit number of working cross-section library
T	Problem title containing 80 characters

RECORD 3: V,R

V(IM)	Volumes of the spatial mesh cells (single-precision)
R(IM+1)	Boundaries of the spatial mesh cells (single-precision)

RECORD 4: W,PNC

W(MM)	Weights in the angular quadrature (single-precision)
PNC(MM,JT)	Scattering constants used to obtain flux moments from angular fluxes (single-precision)

RECORD 5: MA,MZ

MA(IM)	Zone number by interval
MZ(IZM)	Mixture number by zone

RECORD 6: MB,MC,XMD

MB(MS)	Mixture number in the cross-section mixing table
MC(MS)	Component(nuclide) in the cross-section mixing table
XMD(MS)	Atom density in the cross-section mixing table (single-precision)

RECORD 7: CHI,FISNU

CHI(IGM,MXX)	χ for each mixture (single-precision)
FISNU(IGM,MXX)	$\overline{\nu}$ times the fission cross section for each mixture (single-precision)

RECORD 8: EIGEN

EIGEN	k_{eff} (single-precision)

NEXT IGM RECORDS: XNDC

XNDC(IM,MM)	Mesh cell centered angular flux for one group (double-precision)

LAST RECORD: TLEAKAGE

TLEAKAGE(IGM)	Total leakage from the system (single-precision)

6.2 XSDRNPM ADJOINT OUTPUT FILE

For an adjoint case, XSDRNPM writes the following unformatted records on unit NTD, containing the following information:

RECORD 1: EIGEN

EIGEN	k_{eff} value (single-precision)

NEXT IGM RECORDS: XNDC

XNDC(IM,MM)	Mesh cell centered angular flux for one group (double-precision)

The adjoint angular fluxes are reversed in direction such that each angular flux is the importance for that direction in the forward case. This reversal is done by using the reflected angle. Also, the records are written in forward order such that the first record corresponds to the highest-energy group.

6.3 VIP1D OUTPUT FILE

VIP1D has no printed output. An unformatted interface file is written on unit 33 with filename ft33f001. This file is read by the LAKE code. This interface file contains the following:

RECORD 1: ISCT,IGM,IZM,NNEUT,MS,NT1,LINES

ISCT	Order of Legendre scattering expansion
IGM	Number of energy groups
IZM	Number of zones
NNEUT	Number of neutron groups
MS	Length of the XSDRNPM mixing table
NT1	Unit number of working cross-section library
LINES	Number of lines of problem description data written on the file. LAKE reads these lines and prints them.

NEXT LINES RECORDS: PRINTOUT

PRINTOUT	132 characters of problem description data

RECORD 2+LINES: MC

MC(MS)	Component(nuclide) in the cross-section mixing table

RECORD 3+LINES: DENOM,EIGENF,MB,XMD,MZ,T

DENOM	The quantity D defined in Eq. (3.3). A single-fission spectrum, χ, for each mixture is used to calculate DENOM (double-precision)
EIGENF	k_{eff} from the forward case (single-precision)
MB(MS)	Mixture number in the cross-section mixing table
XMD(MS)	Atom density in the cross-section mixing table (single-precision)
MZ(IZM)	Mixture number by zone
T	Problem title containing 80 characters (the first 16 characters are used to identify the case on Plots and the SENPRO interface file written by LAKE)

RECORD 4+LINES: TOTPP

TOTPP(IZM,IGM) Term related to T_g in Eq. (3.7) (double-precision)
TOTPP for a zone is T_g summed over all intervals in that zone.

NEXT IZM RECORDS: SCAT

SCAT(IGM,IGM,ISCT+1) Term related to $P^{\ell}_{g,g'}$ in Eqs. (3.10) and (3.11) (double-precision) SCAT for a zone is $P^{\ell}_{g,g'}$ summed over all intervals in that zone. The first dimension of the array is the adjoint group number, the second is the forward group number, and the third represents the scattering expansion. A separate record is written for each zone.

NEXT RECORD: ZONEFLUX

ZONEFLUX(IGM,IZM) Average flux in each zone by group (double-precision)

LAST RECORD: TLEAKAGE

TLEAKAGE(IGM) Total leakage from the system (single-precision)

7 LAKE PROGRAM DESCRIPTION

LAKE is a computer program that calculates sensitivity coefficients and the estimated uncertainty in k_{eff} due to the uncertainties in the basic nuclear data. LAKE is executed by the SCALE control sequence SEN1 to obtain sensitivities and uncertainties for 1-D criticality models analyzed with XSDRNPM. In addition LAKE can also be used with the DORT code to analyze 2-D systems.

LAKE obtains the information needed for the sensitivity and uncertainty calculations from the following unformatted files:

1. An interface file that contains volume-integrated products of forward and adjoint fluxes. The filename for this file is ft33f001. The information on this file is described in Sect. 6. When using the SCALE control sequence SEN1, this file is written by VIP1D.

2. An AMPX-working library containing the multigroup cross sections used in the forward and adjoint transport calculations. When using the SCALE control sequence SEN1, the filename for this file is ft03f001 when cell-weighted cross sections are used, and ft04f001 otherwise.

3. A sensitivity cross-section library written by NITAWL on file ft20f001. When using the SCALE control sequence SEN1, the NITAWL input parameter MCR is set to 1, which causes this library to be written. This library is used to calculate sensitivity coefficients for elastic scattering, inelastic scattering, and (n,2n). If this library is not present, LAKE will run but will produce fewer sensitivity coefficients.

4. A COVERX covariance file with filename ft34f001.

The output from LAKE consists of printed output and a SENPRO interface file written on unit 40 with filename ft40f001. The printed output is described in Sect. 10. The SENPRO interface file was developed by the FORSS project to store sensitivity profiles (coefficients). A formatted sensitivity file is written on unit 41 with filename ft41f001 and is used for plotting sensitivity profiles.

LAKE calculates sensitivity coefficients using the equations described in Sect. 3. Most of the calculations performed by LAKE are done in the main program and a subroutine called LAKE1. Automatic arrays are used extensively in LAKE1. Only a few subroutines are called from LAKE1. The following subroutines are called by LAKE or LAKE1 and are described briefly:

OPNFIL — OPNFIL is a subroutine from the SCALE subroutine library used to open files. It is called to open a new file that contains the printed output and to open the two existing cross-section files ft03f001 (or ft04f001) and ft20f001.

MODZA — MODZA has two arguments. It receives a SCALE nuclide identifier and returns an integer containing the ZA number of the nuclide. For example, if the nuclide identifier is 1092238, the ZA is 92238.

MTLABEL — MTLABEL has two arguments. It receives an ENDF MT number and returns a label. For example, if the MT number is 18, the label is "fission."

ISOTO	ISOTO has two arguments. It receives a ZA number and returns a label. For example, if the ZA number is 26000, the label is "Fe." ISOTO has a list of ZA numbers and labels. If the ZA number requested is not on this list, the ZA number is returned as the label.
ONE	Subroutine ONE reads groupwise cross sections from both the AMPX-working library and the sensitivity library.
TWO	Subroutine TWO reads transfer matrix cross sections from both the AMPX-working library and the sensitivity library.
CCC	CCC writes character strings such that six characters are written in eight-character double words. This subroutine is a relic required to be compatible with FORSS codes that were written to store character data in double-precision variables.
CAVA	Subroutine CAVA is a rewritten version of the CAVALIER module from FORSS. It performs the uncertainty analysis.

8 PLOT PROGRAM DESCRIPTION

PLOT is a computer program that produces postscript plots of sensitivity coefficients. It currently is available only on IBM AIX workstations. Another plotting code SENPLOT has been written for use on Windows 95/98/NT personal computers.

Plots of groupwise sensitivity coefficients per unit lethargy are called sensitivity profiles. In the FORSS system, plots of sensitivity profiles were made using the SENPRO service module. This module has been rewritten for use on IBM AIX workstations. The main modification was to remove the outdated plotting method and use the PLPLOT package that was already installed on the Computation Physics and Engineering Division workstations at ORNL. Another modification was to make the plotting code run without user input by choosing suitable defaults for the size of the plots. A postscript output file is written that contains a plot for every nuclear reaction where the sum of the absolute value of the groupwise sensitivity coefficients is greater than 0.005. The sensitivity interface file on unit 41 is read, and a plot file named plot.ps is written. It is not necessary to save the plot.ps file since it may be easily created later provided file ft41f001 is saved. File ft41f001 is always much smaller than file plot.ps.

Several examples of sensitivity-profile plots are shown in Sect. 11. These plots are for the UF_4 problem described there. The information printed above the plot is the 16-character title obtained from the title card of the SEN1 case, the nuclear reaction (isotope and reaction), and the energy-integrated sensitivity coefficient. The plots use the convention of having solid lines for negative sensitivity coefficients and a dashed line for positive sensitivity coefficients. When both positive and negative groupwise sensitivities are present in the same profile, a quantity called "OSC," which stands for opposite sign contribution, is printed to the right of the plot. This situation is demonstrated by the first plot in Sect. 11. This plot shows the sensitivity coefficients for the total cross section of ^{19}F. The OSC value is −3.1606 E-3, which is the sum of all negative groupwise sensitivity coefficients.

9 SEN1 INPUT DESCRIPTION

The input to SEN1 consists of a SCALE Analytical Sequence Specification Record, SCALE Material Information Processor data, and criticality problem data. No additional input is required to obtain sensitivity and uncertainty results. The data for each of these segments are entered using the SCALE free-form reading routines. The input is not case sensitive, so either upper- or lowercase letters may be used. A maximum of 80 columns per line may be used for input.

9.1 ANALYTICAL SEQUENCE SPECIFICATION RECORD

The analytical sequence specification begins in column 1 of the first line of the input file and must contain either

=SEN1 when INFHOMMEDIUM or MULTIREGION (no cell-weighting) is specified for the type of calculation in the material input processor data to follow, or

=SEN1X when MULTIREGION or LATTICECELL is specified for the type of calculation in the material input processor data in order to obtain cell-weighted cross sections.

Optional keyword input may be entered, starting after column 10 of the analytical sequence specification record. These keywords are

PARM=CHECK
PARM=CHK This option allows the input data to be read and checked without executing any functional modules.

PARM=SIZE=n The amount of memory requested in four-byte words may be set with this entry. The default value for n is 1000000.

PARM=(CHECK,SIZE=n) This option allows checking and size specification.

9.2 MATERIAL INPUT PROCESSOR DATA

The material input processor data are exactly the same as that used in CSAS, SAS1, and other SCALE control modules. See Table 9.1 for an input description. More detailed descriptions of this input are found in Sect. C4.4 of the SCALE document. The first line of material input processor input is a title. The title can contain up to 80 characters. The first 16 characters of the title are written on the SENPRO interface file and are used to label sensitivity-profile plots.

9.3 CRITICALITY PROBLEM DATA

The criticality problem data are used by the SEN1 control sequence to prepare input for the forward and adjoint XSDRNPM criticality cases needed to calculate cross-section sensitivities. The criticality problem data consist of the following items:

Table 9.1 Tables of Material Information Processor data requirements

Outline of standard compositions specification data

Entry No.	Variable name	Type of data	Entry requirement	Comments
1	SC	Standard composition component name	Always	Enter once for each standard composition. Enter the alphanumeric description from Sect. M8.2. Additional allowed names include those beginning with ARBM for arbitrary materials, and SOLN for solutions
A1	ROTH	Theoretical density of material (g/cc)	ARBM	Enter once for each arbitrary material
A2	NEL	Number of elements or nuclides in the material	ARBM	Enter once for each arbitrary material
A3	IVIS	No longer used but must still be entered	ARBM	Enter once for each arbitrary material. Enter 0 or 1
A4	ICP	Compound indicator	ARBM	Enter once for each arbitrary material. Enter 1 for a chemical compound, 0 for alloys, mixtures, etc.
A5	IRS	No longer used but must still be entered	ARBM	Enter once for each standard composition component that is an arbitrary material. Enter 0 or 1
A6	NCZA	ID number (from far right column of Table M8.2.1 or M8.2.2)	ARBM	Repeat the sequences A6 and A7 for each element in the arbitrary material before entering entry number 2. Enter the number from the far right column of Table M8.2.1 or M8.2.2. (Premixed standard compositions cannot be used in an arbitrary material definition.)
A7	ATPM	Number of atoms of this element per molecule of arbitrary material	ARBM and ICP = 1	Repeat the sequence A6 and A7 for each element in the arbitrary material before entering entry number 2. Do not enter a value unless ICP = 1
		or	or	or
		Weight percent of this element in this arbitrary material	ARBM and ICP = 0	Repeat the sequence A6 and A7 for each element in the arbitrary material before entering entry number 2. Do not enter a value unless ICP = 0

Table 9.1 (continued)

Outline of standard compositions specification data (continued)

Entry No.	Variable name	Type of data	Entry requirement	Comments
2	MX	Mixture ID number	Always	Enter once for each standard composition component
S1	FD	Fuel density (grams of U or Pu per liter of solution)	SOLN	Enter once for a solution
S2	AML	Acid molarity of the solution	SOLN	Enter once for a solution. AML = 0 if there is no acid in the solution
O1	SPGR or ROTH	Specific gravity of the solution or Density of the basic standard composition	Optional	If the specific gravity (SPGR) of the solution is known, it should be entered as SPG = SPGR or If the density of a basic standard composition (ROTH) is to be entered, use DEN = ROTH
3	VF	Density multiplier	See comment column	Enter the density multiplier (density fraction, volume fraction, or a combination). Default value is 1. This item can be omitted if entries 4, 5, 6a, and 6b are also omitted. VF = 0 is not allowed for SOLN or ARBM
4	ADEN	Number density (atoms/b-cm) for the nuclide	VF = 0	Enter only if VF = 0.0
5	TEMP	Temperature (K)	See comment column	Default value is 293 K. This entry can be omitted if entries 6a and 6b are also omitted
6a	IZA	Isotope's ZA number	VF ≠ 0	Enter for each isotope in a multiple isotope nuclide. Omit if VF = 0. Entries 6a and 6b are entered in pairs until each isotope in the nuclide is defined
6b	WTP	Weight percent of the isotope	VF ≠ 0	Enter for each isotope in a multiple-isotope nuclide. Omit if VF = 0.0. Entries 6a and 6b are entered in pairs until each isotope in the nuclide is defined
7*	END	Terminate a standard composition	Always	Enter once for each standard composition component. This terminates the data for a standard composition component. Enter END to terminate the component. Repeat entries 1 through 7 until all the mixtures have been defined. At least two blanks must separate entry 7 from the next entry
	END COMP	Terminate the data block	Terminus	Enter once for a problem. Enter the words END COMP when all the standard composition components have been described. At least two blanks must follow the END COMP

*Entry 7 should not begin in column 1 unless a name is associated with it.
At least two blanks should separate the last entry 7 from the END COMP.

.

Table 9.1 (continued)

Optional unit cell specifications for INFHOMMEDIUM problems

Entry No.	Variable name	Type of data	Data entry	Comments
1	NAME	Keyword	CELLMIX	Initiate reading cell data for INFHOMMEDIUM
2	MFUEL	Mixture number in the cell	Mixture number	Specifies the mixture number to be used in the cell. Defaults to the smallest mixture number entered in the Standard Composition Data

Unit cell data are necessary for INFHOMMEDIUM only if a mixture number other than the smallest mixture number is to be used in the cell and a control sequence that executes XSDRNPM has been specified. If mixtures 1, 2, and 3 are specified and mixture 3 is to be used in the cell, enter CELLMIX 3.

Unit cell specification for LATTICECELL problems

Entry No.	Variable name	Type of data	Entry requirement	Data entry	Comments
1	CTP	Type of lattice	Always		Describes the type of lattice or array configuration
				SQUAREPITCH	Use for cylindrical rods in a square pitch
				ASQUAREPITCH	Use for annular cylindrical rods in a square pitch
				ASQP	Use for annular cylindrical rods in a square pitch
				TRIANGPITCH	Use for cylindrical rods in a triangular pitch
				ATRIANGPITCH	Use for annular cylindrical rods in a triangular pitch
				ATRP	Use for annular cylindrical rods in a triangular pitch
				SPHSQUAREP	Use for spherical pellets in a cubic lattice
				ASPHSQUAREP	Use for annular spherical pellets in a cubic lattice
				ASSP	Use for annular spherical pellets in a cubic lattice
				SPHTRIANGP	Use for spherical pellets in a bi-centered or face centered hexagonal close-packed lattice
				ASPHTRIANGP	Use for spherical pellets in a bi-centered or face centered hexagonal close-packed lattice
				ASTP	Use for spherical pellets in a bi-centered or face centered hexagonal close-packed lattice
				SYMMSLABCELL	Use for a symmetric array of slabs
				ASYMSLABCELL	Use for a periodic, but asymmetric array of slabs
2	PITCH	Array pitch (cm)	Always	Appropriate dimension	The center-to-center spacing (cm) between fuel lumps. For asymmetric slab cell, enter the distance from the center of one moderator to the center of the other moderator (cm)

Table 9.1 (continued)

Unit cell specification for LATTICECELL problems (continued)

Entry No.	Variable name	Type of data	Entry requirement	Data entry	Comments
3	FUELOD	Outside dimension of fuel (cm)	Always	Appropriate dimension	Outside diameter of fuel (cm), or the thickness of the fuel in a slab
4	MFUEL	Fuel mixture number	Always	Mixture number	Mixture number representing the fuel
5	MMOD	Moderator mixture number	Always	Mixture number	Mixture number representing the moderator
6	MMOD2	2nd moderator mixture number	Annular cell	Mixture number	Mixture number representing the second moderator
7	TKMOD2	2nd moderator thickness or 2nd moderator diameter (cm)	ASYMSLAB CELL or annular cell	Thickness or Diameter	Thickness of the second moderator (cm) for ASYMSLABCELL or Diameter of inner moderator (cm) for other annular cells
8	CLADOD	Outside diameter of clad (cm)	If clad	Clad OD	OMIT IF NO CLAD. For a slab, CLADOD is the sum of thickness of the fuel, gap, and clad
9	MCLAD	Clad mixture number	If clad	Mixture number	OMIT IF NO CLAD. Mixture number representing the clad
10	CLADID	Inside diameter of clad (cm)	If gap	Clad ID	OMIT IF NO GAP between the fuel and clad
11	MGAP	Gap mixture number	If gap	Mixture number	OMIT IF NO GAP between the fuel and clad A mixture number of zero is often used
12	END	Terminate LATTICECELL data	Always	END	Terminate the LATTICECELL input data by entering the word END. Do not start in column 1. At least two blanks must follow entry No. 12

Table 9.1 (continued)

Unit cell specification for MULTIREGION problems

Entry No.	Variable name	Type of data	Entry requirement	Data entry	Comments
1	CS	Type of geometry	Always		Describes the type of geometry. The options are listed below
				SLAB	Use for slab geometry
				CYLINDRICAL	Use for cylindrical geometry
				SPHERICAL	Use for spherical geometry
				BUCKLEDSLAB	Use for slab geometry with a buckling correction for the two transverse directions
				BUCKLEDCYL	Use for cylindrical geometry with a buckling correction in the axial direction
2	BR	Right boundary condition	Required for BUCKLEDSLAB and BUCKLEDCYL		Default is VACUUM. Describes the right/outside boundary condition
				VACUUM	Provides a nonreturn condition at the boundary
			Optional for other geometries	REFLECTED	Do not use for cylindrical or spherical
				PERIODIC	Do not use for cylindrical or spherical
				WHITE	Provides isotopic return at the boundary
3	BL	Left boundary condition	Required for BUCKLEDSLAB and BUCKLEDCYL		Default is REFLECTED. Describes the left boundary condition
				VACUUM	Provides a nonreturn condition at the boundary
			Optional for other geometries	REFLECTED	Recommended for cylindrical or spherical
				PERIODIC	Do not use for cylindrical or spherical
				WHITE	Provides isotropic return at the boundary
4	ORGN	Location of left boundary on the x-axis (cm)	BUCKLEDSLAB and BUCKLEDCYL Optional for other geometries	Appropriate dimension	Default is 0.0. Should not be changed for cylindrical or spherical geometry A value must be entered if subsequent data are to be entered
5	DY	Buckling height (cm)	BUCKLEDSLAB and BUCKLEDCYL	Appropriate dimension	OMIT FOR SLAB, CYLINDRICAL, and SPHERICAL Corresponds to one of the transverse dimensions of an actual 3-D slab assembly or to the length of a finite cylinder
6	DZ	Buckling depth (cm)	BUCKLEDSLAB	Appropriate dimension	OMIT UNLESS BUCKLEDSLAB WAS SPECIFIED Buckling depth corresponding to the second transverse dimension of a 3-D slab assembly
7	END	End geometry parameters	Always	END	Enter the word END. Do not start in column 1. At least two blanks must separate entry 7 from the first entry 8
8	MXZ	Mixture number in the zone	Always	Mixture number	Repeat entry numbers 8-10 until all zones are defined Enter the mixture number for this zone

Table 9.1 (continued)

Unit cell specification for MULTIREGION problems (continued)

Entry No.	Variable name	Type of data	Entry requirement	Data entry	Comments
9	RZ	Outside radius of the zone (cm)	Always	Appropriate dimension	Repeat entry numbers 8–10 until all zones are defined. Enter the outside dimension of the zone (cm)
10	XMOD	External moderator index	Optional		Repeat entry numbers 8–10 until all zones are defined Entry 10 is optional and can be omitted. If it is omitted, repeat entry numbers 8 and 9 until all zones are defined
				NOEXTERMOD	No moderating materials in the adjacent zones
				ONEEXTERMOD	A moderating material is present in one adjacent zone
				TWOEXTERMOD	Moderating materials are present in two adjacent zones
	END ZONE	Terminate zone data		END ZONE	Enter when all zones have been defined by repeating entry numbers 8 through 10 for each zone. At least two blanks must follow this entry

Table 9.1 (continued)

Summary of available optional parameter data

Entry No.	Keyword name	Type of data	Applicable module	Comments
1	MORE DATA	Input flag		This signals that optional parameter data will be entered Enter only those parameters you wish to change
2	ISN=	Order of angular quadrature	XSDRNPM	The default value is 8. Allows using another value
3	SZF=	Spatial mesh size factor	XSDRNPM	The default value is 1.0. 0<SZF<1.0 gives a finer mesh SZF>1.0 gives a coarser mesh
4	IIM=	Max. number of inner iterations	XSDRNPM	The default value is 20. Allows using another value
5	ICM=	Max. number of outer iterations	XSDRNPM	The default value is 25. Allows using another value
6	EPS=	Overall convergence criteria	XSDRNPM	The default value is 0.0001. Allows using another value
7	PTC=	Point convergence criteria	XSDRNPM	The default value is 0.0001. Allows using another value
8	BKL=	Buckling factor	XSDRNPM	The default value is 1.420892. Use ONLY for a MULTIREGION problem that specifies BUCKLEDSLAB or BUCKLEDCYL
9	IUS=	Upscatter scaling factor	XSDRNPM	The default value is zero. IUS=0 doesn't utilize upscatter scaling. IUS=1 uses upscatter scaling to accelerate the solution and/or speed convergence
10	RES=	Resonance data	BONAMI NITAWL	Enter the mixture number, geometry type (SLAB, CYLINDER, SPHERE) and the thickness of the slab or radius of the sphere or cylinder, in cm. Optionally enter the inner radius (cm) to specify an annular cylinder or sphere
11	DAN(mm)=	Dancoff factor for the specified mixture	BONAMI NITAWL	Enter the mixture number, mm, to which the Dancoff factor applies inside the parentheses; enter the Dancoff factor after the equal sign
NOTE: Repeat entry numbers 10 and 11 for all resonance mixtures used in the problem that are not treated in the LATTICECELL or MULTIREGION description				
12	BAL=	Key to print balance tables	XSDRNPM	The default value is FINE. BAL=NONE suppresses printing the balance table. BAL=ALL prints all balance tables. BAL=FINE prints only the fine-group balance tables
13	DY=	First transverse dimension	XSDRNPM	The first transverse dimension, in cm, used in a buckling correction to calculate leakage normal to the principal calculation direction (i.e., the height of a slab or a cylinder)
14	DZ=	Second transverse dimension	XSDRNPM	The second transverse dimension in centimeters used for a buckling correction (i.e., the width of a slab)
15	COF=	Diffusion coefficient option for transverse leakage corrections	XSDRNPM	The default is 0. See Sect. F3.5, 3$ array, variable IPN
16	FRD=	Unit from which fluxes will be read	XSDRNPM	Enter the unit number from which the flux guess for XSDRNPM will be read

Table 9.1 (continued)

Summary of available optional parameter data (continued)

Entry No.	Keyword name	Type of data	Applicable module	Comments
17	FWR=	Unit on which fluxes will be written	XSDRNPM	Enter the unit number where the binary fluxes from XSDRNPM will be written
18	ADJ=	Adjoint mode flag	XSDRNPM	Enter a 1 to cause XSDRNPM to solve the problem in adjoint mode
19	NBU=	Unit on which balance tables will be written	XSDRNPM	Enter the unit number where the balance tables from XSDRNPM will be written
20	WGT=	Cross-section weighting flag	XSDRNPM	Enter a 0 to suppress doing the cross-section weighting in XSDRNPM
21	ZMD(iz)=	Zone width modifier for the specified zone	XSDRNPM	Enter the zone number for which the modifier applies inside the parentheses; enter the zone width modifier after the equal sign. **Repeat number 20 to specify all zones to be modified in a search**
22	INT(iz)=	Number of intervals for the specified zone	XSDRNPM	Enter the zone number inside the parentheses; enter the number of intervals after the equal sign. Repeat number 22 to specify all needed zones
23	KEF=	Value of k_{eff} to be searched for	XSDRNPM	Enter the value of k_{eff} that it is desired to find. The default is 1.0
24	KFM=	Value of the eigenvalue modifier	XSDRNPM	Enter the value of the eigenvalue modifier (i.e., the relative change for the first guess of a search). The default is -0.1
25	DAB=	Number of direct-access data blocks	MIP*	The default is 200. Number of blocks allocated for direct-access unit 90
26	AXS=	Unit on which a mixed ANISN library will be written	ICE	Enter the unit number where ICE is to write a mixed ANISN library
27	MSH=	Maximum number of mesh points/resonance	NITAWL	The default value is 2001. Allows using another value
28	MLV=	Highest resonance ℓ-value for self-shielding	NITAWL	The default value is 2. Allows using another value
29	ID1=	Print control for scalar fluxes	XSDRNPM	The default value is -1. See Sect. F3.5, 2$ array, variable ID1
30	COLL	Key to activate collapse of thermal groups	MIP[a]	Enter COLL to collapse all thermal groups into one group for the shielding sequences
31	END	Terminus		Terminate the optional parameter data. Do not start in column 1. **At least two blanks must follow this entry**

*MIP is the Material Information Processor.

1. A line containing the geometry and boundary conditions for the XSDRNPM criticality case. The first entry on this line describes the geometry and must be SLAB, CYLINDRICAL, or SPHERICAL. The second entry is optional and describes the right-boundary condition. The default value for the right-boundary condition is VACUUM. The third entry on this line is optional and describes the left-boundary condition. The default value for the left-boundary condition is REFLECTED. The last entry on this line is END. Valid entries for the boundary conditions are the following:

   VACUUM - No return at boundary
   REFLECTED - Specular (mirror-like) return at boundary
   PERIODIC - Infinite array of cells in slab geometry
   WHITE - Isotropic return at boundary

2. A line containing the following three entries for each zone of the XSDRNPM case:

   a. mixture number in the zone,
   b. outer zone dimension (in cm), and
   c. number of equally spaced mesh intervals in the zone.

   The mixture numbers are defined in the material input processor input. Mixture 0 is used for voids, and mixture 500 is used for the cell-weighted mixture when =SEN1X is specified on the analytical sequence specification record. The left (inner) dimension of the first zone is zero.

3. A line containing END ZONE.

4. Optional line or lines that contain entries for selected XSDRNPM input parameters. A list of the parameters and their default values are found in Table 9.2.

5. A line containing STOP.

6. A line containing END in column 1. This END terminates the SEN1 SCALE control sequence.

Figures 9.1 and 9.2 show examples of SEN1 input using the unit-cell calculation types INFHOMMEDIUM and LATTICECELL, respectively, for the material input processor. The SEN1 sample problem in the next section uses the unit-cell calculation type MULTIREGION.

Table 9.2 Optional parameter input for the criticality problem data

Name	Default	Meaning
ISN=	16	Order of angular quadrature
IIM=	20	Inner-iteration maximum
ICM=	100	Outer-iteration maximum
ID1=	-1	Flux-edit option:
		-1 no flux print 0 scalar flux print 1 scalar and angular flux print
SCT=	3	Order of Legendre expansion for cross sections
PRT=	-2	Cross-section print option:
		-2 no cross-section print -1 print 1-D cross sections 0/N print 2-D cross sections through order N
PBT=	0	Balance table print option:
		-1 no balance table print 0 fine group balance table print
EPS=	1.E-6	Outer-iteration convergence criteria
PCT=	1.E-6	Inner-iteration convergence criteria
DY=	0	First-transverse dimension (cm) for buckling correction
DZ=	0	Second-transverse dimension (cm) for buckling correction

```
=sen1
U(2)F4 H/X=294  raffety and milhalczo u(2)f4-2 unreflected (case 14)
44group         infhommedium
u-235  1 0 1.3303e-4 end
u-238  1 0 6.4370e-3 end
h      1 0 3.9097e-2 end
c      1 0 1.8797e-2 end
f      1 0 2.6280e-2 end
end comp
spherical  end
1 38.50 160
end zone
isn=8
stop
end
```

Figure 9.1 Example SEN1 input for infhommedium cross-section preparation

```
=sen1x
u(10)o2 p=.7 1-d  leu-comp-therm-032  case 1
44groupndf5                  latticecell
u-234          1  0.0 1.7636e-5 293 end
u-235          1  0.0 2.1577e-3 293 end
u-236          1  0.0 1.53e-5 293 end
u-238          1  0.0 1.951e-2 293 end
o              1  0.0 4.4661e-2 293 end
fe             2  0.0 5.8894e-2 293 end
cr             2  0.0 1.6469e-2 293 end
ni             2  0.0 8.1061e-3 293 end
si             2  0.0 1.3551e-3 293 end
mn             2  0.0 1.299e-3 293 end
c              2  0.0 2.3766e-4 293 end
ti             2  0.0 4.4713e-4 293 end
h2o            3  1.0 293 end
h2o            4  1.0 293 end
end comp
triangpitch .7 .416 1  3  .51 2  .43 0  end
cylindrical   end
500 16.44 32
4   46.44 30
end zone
isn=10
stop
end
```

Figure 9.2 Example SEN1 input for latticecell cross-section preparation

10 SAMPLE PROBLEM AND OUTPUT DESCRIPTION

The sample problem is the Flattop-25 metal system from the Cross-Section Evaluation Working Group benchmark specifications.[5] The system consists of a 6.116-cm sphere of 93%-enriched uranium with a natural uranium reflector. The outer radius of the reflector is 24.13 cm. The input for this problem is shown in Figure 10.1.

The output of the LAKE sensitivity code is shown in Figure 10.2. The first line of output is the title. Plots will identify the system as Flattop-25.

The next ten lines of output contain integers that describe various characteristics of the transport calculations such as the number of neutron groups and the angular quadrature order.

Next the values of k_{eff} from the forward and adjoint cases and the differences between them are printed. This difference provides a measure of the quality of the transport calculations. For all cases studied to date, this difference was reduced to 1.E-4 or smaller by refining the spatial mesh and/or the order of the angular quadrature. Table 10.1 illustrates this point by showing how the difference between the forward and adjoint values of k_{eff} varies as the quadrature order is increased. Note that the k_{eff} difference is somewhat smaller than the change in k_{eff} obtained by increasing the order of the quadrature.

The next part of the output shows energy-integrated sensitivities on a zone and nuclide basis. This information is printed in the order that the nuclides are written on the AMPX working library (the sensitivity library has the same nuclides in the same order as the working library). Three pieces of information from the working library are printed from the directory records of the working library to identify the nuclide:

1. a nuclide symbol (four characters of text),

2. an identifier of the set (the rightmost five digits are the ZA number), and

3. 72 characters of text describing the set.

After this header information, the energy-integrated sensitivities are printed for each zone containing the nuclide, along with the number density of the nuclide in that zone.

The next information printed is a summary of sensitivities. This summary contains the sensitivities for each ZA number and is obtained by summing the previously printed information over zone. As previously mentioned in Sect. 4, this summary is an approximation because the sensitivities are actually the sensitivities of changing the shielded cross sections, and different shielded cross sections are used for zone 1 and zone 2 of the sample problem. The groupwise sensitivity coefficients corresponding to the energy-integrated values printed are written on units 40 and 41. They are used for the following uncertainty analysis and are plotted. At the bottom of this summary is the sum of the $\bar{\nu}$ sensitivity coefficients over all nuclides. For the sample problem the value is very close to 1.0, as it has been for every system studied to date.

```
=sen1
flattop-25       benchmark, 44-grp cross sections
44gr multiregion
u-234   1  0.0  4.90-4  end
u-235   1  0.0  4.449-2  end
u-238   1  0.0  2.70-3  end
u-235   2  0.0  3.40-4  end
u-238   2  0.0  4.774-2  end
end comp
spherical    end
1  6.116
2  24.13
end zone
spherical    end
1  6.116 120
2  24.13 120
end zone
isn=32
stop
end
```

Figure 10.1 SEN1 sample problem for Flattop-25

```
flattop-25       benchmark, 44-grp cross sections

          44   number of neutron groups
           0   number of gamma groups
          32   s(n) quadrature order
           3   p(l) order of scattering
         240   number of spatial intervals
           2   number of spatial zones
           5   length of mixing table
           3   ½/3 = plane/cylinder/sphere
           1   left boundary condition  0/1/2/3 = vacuum/refl/per/white
           0   right boundary condition
    0.997118   k-eff from the forward case
    0.997084   k-eff from the adjoint case
    0.000034   (forward - adjoint) k-eff

 u 38   1092238   92U 238 ANL+ EVALJUN77 E.PENNINGTON A.           MOD3 02/13/92

zone=   1  number density=  2.7000E-03    U-238  total      a=  8.0969E-03
zone=   1  number density=  2.7000E-03    U-238  scatter    a=  4.2734E-03
zone=   1  number density=  2.7000E-03    U-238  elastic    a=  2.2790E-03
zone=   1  number density=  2.7000E-03    U-238  n,n'       a=  1.9215E-03
zone=   1  number density=  2.7000E-03    U-238  n,2n       a=  7.2218E-05
zone=   1  number density=  2.7000E-03    U-238  fission    a=  5.4430E-03
zone=   1  number density=  2.7000E-03    U-238  capture    a= -1.6195E-03
zone=   1  number density=  2.7000E-03    U-238  n,gamma    a= -1.6195E-03
zone=   1  number density=  2.7000E-03    U-238  nubar      a=  8.2149E-03
zone=   1  number density=  2.7000E-03    U-238  chi        a=  8.2149E-03

 u 38   2092238   92U 238 ANL+ EVALJUN77 E.PENNINGTON A.           MOD3 02/13/92

zone=   2  number density=  4.7740E-02    U-238  total      a=  2.1621E-01
zone=   2  number density=  4.7740E-02    U-238  scatter    a=  1.9812E-01
zone=   2  number density=  4.7740E-02    U-238  elastic    a=  1.3228E-01
zone=   2  number density=  4.7740E-02    U-238  n,n'       a=  6.5217E-02
zone=   2  number density=  4.7740E-02    U-238  n,2n       a=  6.3279E-04
zone=   2  number density=  4.7740E-02    U-238  fission    a=  5.9224E-02
zone=   2  number density=  4.7740E-02    U-238  capture    a= -4.1131E-02
zone=   2  number density=  4.7740E-02    U-238  n,gamma    a= -4.1131E-02
zone=   2  number density=  4.7740E-02    U-238  nubar      a=  8.2944E-02
zone=   2  number density=  4.7740E-02    U-238  chi        a=  8.2944E-02

 u 34   1092234   92U 234 BNL HEDL + EVALJUL78 DIVADEENAM MANN     MOD3 01/10/91

zone=   1  number density=  4.9000E-04    U-234  total      a=  5.0306E-03
zone=   1  number density=  4.9000E-04    U-234  scatter    a=  7.8110E-04
zone=   1  number density=  4.9000E-04    U-234  elastic    a=  5.0965E-04
zone=   1  number density=  4.9000E-04    U-234  n,n'       a=  2.7049E-04
zone=   1  number density=  4.9000E-04    U-234  n,2n       a=  1.1694E-06
zone=   1  number density=  4.9000E-04    U-234  fission    a=  4.9122E-03
zone=   1  number density=  4.9000E-04    U-234  capture    a= -6.6265E-04
zone=   1  number density=  4.9000E-04    U-234  n,gamma    a= -6.6265E-04
zone=   1  number density=  4.9000E-04    U-234  nubar      a=  7.4355E-03
zone=   1  number density=  4.9000E-04    U-234  chi        a=  7.4355E-03
```

Figure 10.2 LAKE output for the sample problem

```
 u 35   1092235   92u 235 bnl evalapr77 m.r.bhat                  mod3 02/28/89

zone=   1  number density=  4.4490E-02    U-235  total      a=  5.8378E-01
zone=   1  number density=  4.4490E-02    U-235  scatter    a=  5.9466E-02
zone=   1  number density=  4.4490E-02    U-235  elastic    a=  3.6955E-02
zone=   1  number density=  4.4490E-02    U-235  n,n'       a=  2.1723E-02
zone=   1  number density=  4.4490E-02    U-235  n,2n       a=  7.8935E-04
zone=   1  number density=  4.4490E-02    U-235  fission    a=  5.6783E-01
zone=   1  number density=  4.4490E-02    U-235  capture    a= -4.3515E-02
zone=   1  number density=  4.4490E-02    U-235  n,gamma    a= -4.3515E-02
zone=   1  number density=  4.4490E-02    U-235  nubar      a=  8.9063E-01
zone=   1  number density=  4.4490E-02    U-235  chi        a=  8.9063E-01

 u 35   2092235   92u 235 bnl evalapr77 m.r.bhat                  mod3 02/28/89

zone=   2  number density=  3.4000E-04    U-235  total      a=  8.3346E-03
zone=   2  number density=  3.4000E-04    U-235  scatter    a=  1.2326E-03
zone=   2  number density=  3.4000E-04    U-235  elastic    a=  9.4054E-04
zone=   2  number density=  3.4000E-04    U-235  n,n'       a=  2.8947E-04
zone=   2  number density=  3.4000E-04    U-235  n,2n       a=  2.5786E-06
zone=   2  number density=  3.4000E-04    U-235  fission    a=  7.6923E-03
zone=   2  number density=  3.4000E-04    U-235  capture    a= -5.9036E-04
zone=   2  number density=  3.4000E-04    U-235  n,gamma    a= -5.9036E-04
zone=   2  number density=  3.4000E-04    U-235  nubar      a=  1.0819E-02
zone=   2  number density=  3.4000E-04    U-235  chi        a=  1.0819E-02

summary of sensitivities

   92234    U-234  total      a=  5.0306E-03
   92234    U-234  scatter    a=  7.8110E-04
   92234    U-234  elastic    a=  5.0965E-04
   92234    U-234  n,n'       a=  2.7049E-04
   92234    U-234  n,2n       a=  1.1694E-06
   92234    U-234  fission    a=  4.9122E-03
   92234    U-234  capture    a= -6.6265E-04
   92234    U-234  n,gamma    a= -6.6265E-04
   92234    U-234  nubar      a=  7.4355E-03
   92234    U-234  chi        a=  7.4355E-03
   92235    U-235  total      a=  5.9211E-01
   92235    U-235  scatter    a=  6.0699E-02
   92235    U-235  elastic    a=  3.7895E-02
   92235    U-235  n,n'       a=  2.2012E-02
   92235    U-235  n,2n       a=  7.9193E-04
   92235    U-235  fission    a=  5.7552E-01
   92235    U-235  capture    a= -4.4105E-02
   92235    U-235  n,gamma    a= -4.4105E-02
   92235    U-235  nubar      a=  9.0145E-01
   92235    U-235  chi        a=  9.0145E-01
   92238    U-238  total      a=  2.2431E-01
   92238    U-238  scatter    a=  2.0239E-01
   92238    U-238  elastic    a=  1.3456E-01
   92238    U-238  n,n'       a=  6.7138E-02
   92238    U-238  n,2n       a=  7.0501E-04
   92238    U-238  fission    a=  6.4667E-02
   92238    U-238  capture    a= -4.2751E-02
   92238    U-238  n,gamma    a= -4.2751E-02
   92238    U-238  nubar      a=  9.1159E-02
   92238    U-238  chi        a=  9.1159E-02

    1.000041   sum of nubar sensitivities
```

Figure 10.2 (continued)

```
  problem characterization


 median fission group is    9    1.400E+06 to 9.000E+05(eV)
                          average fission group   8.341E+00
             average energy(eV) causing fission   1.653E+06
 energy(eV) of average lethargy causing fission   8.419E+05

 median capture group is   11    4.000E+05 to 1.000E+05(eV)
                          average capture group   1.098E+01
                  average energy(eV) of capture   3.866E+05
      energy(eV) of average lethargy of capture   1.682E+05

 median scatter group is   11    4.000E+05 to 1.000E+05(eV)
                          average scatter group   1.040E+01
                  average energy(eV) of scatter   6.102E+05
      energy(eV) of average lethargy of scatter   2.649E+05

 median leakage group is   11    4.000E+05 to 1.000E+05(eV)
                          average leakage group   1.047E+01
                  average energy(eV) of leakage   5.532E+05
      energy(eV) of average lethargy of leakage   2.803E+05
```

Figure 10.2 (continued)

```
  the standard deviation of keff is:
   1.795    percent

   contributions *10**4 by reaction pairs to the
   relative covariances of k-eff

            diagonal                off-diagonal

 U-235  fission   1.226E+00
 U-235  n,gamma   6.578E-01
 U-238  total     3.553E-01
                              U-238  elastic   9.829E-02
                              U-238  n,n'      8.478E-02
                              U-238  n,gamma   4.399E-08
                              U-238  fission  -3.905E-16
 U-235  nubar     2.529E-01
 U-238  n,n'      2.304E-01
                              U-238  total     8.478E-02
                              U-238  elastic  -5.551E-02
                              U-238  fission  -1.896E-03
                              U-238  n,gamma   3.452E-04
                              U-238  n,2n     -1.868E-05
 U-238  elastic   1.873E-01
                              U-238  total     9.829E-02
                              U-238  n,n'     -5.551E-02
                              U-238  n,gamma   1.863E-03
                              U-238  fission  -5.734E-06
 U-238  n,gamma   3.780E-02
                              U-238  elastic   1.863E-03
                              U-238  n,n'      3.452E-04
                              U-238  total     4.399E-08
 U-238  fission   1.899E-02
                              U-238  n,n'     -1.896E-03
                              U-238  elastic  -5.734E-06
                              U-238  total    -3.905E-16
 U-238  n,2n      3.946E-05
                              U-238  n,n'     -1.868E-05
 U-238  nubar     0.000E+00
```

Figure 10.2 (continued)

Table 10.1 Values of k_{eff} for different angular quadratures

	S-8	S-16	S-32
k_{eff} from the forward case	1.000084	0.997837	0.997221
k_{eff} from the adjoint case	0.999622	0.997707	0.997187
(Forward - adjoint) k_{eff}	0.000462	0.000129	0.000034

The next section of the printout contains several parameters that characterize the problem. Some of these parameters have been used previously by criticality safety analysts to compare systems. The four parameters printed for fission are the following:

1. Median fission group and the energy boundaries of that group

2. Average fission group (KENO output contains this parameter)

3. Average energy-causing fission

4. Energy of average lethargy-causing fission (KENO output contains this parameter)

The median fission group is the group where half of all fissions occur either in this group or in higher-energy groups.

Information similar to that printed for fission is also printed for capture, scattering, and leakage.

The final printed information describes the uncertainty calculation. First, the calculated standard deviation (uncertainty) in k_{eff} is printed. Next, the individual contributions to the uncertainty are printed. The column labeled diagonal refers to uncertainties from covariance matrices for a single nuclear reaction. The off-diagonal column refers to uncertainties from covariance matrices for two different reactions.

11 VERIFICATION

A simple spherical model of an actual critical experiment was chosen to study in order to verify that the calculated sensitivities are correct. The SEN1 input file used to perform the sensitivity calculation is shown in Figure 9.1. The energy-integrated sensitivity coefficients calculated by LAKE are shown in Table 11.1. Plots of selected ^{19}F sensitivity coefficients are shown in Figures 11.1–11.6.

A number of consistency checks can be performed:

1. The total sensitivity for each isotope should equal the sum of the scattering, capture, and fission sensitivities.

2. The capture sensitivity should almost equal the sum of all of the individual capture reactions such as (n,γ) or (n,α).

3. The scattering sensitivity should almost equal the sum of elastic, inelastic, and (n,2n) sensitivities. Inelastic is denoted by (n,n') in the table and in the output of LAKE.

4. The fission sensitivity should be less than the $\bar{\nu}$ sensitivity.

5. The energy-integrated $\bar{\nu}$ sensitivity should equal the energy-integrated χ sensitivity.

6. The sum of the energy-integated $\bar{\nu}$ sensitivities over all nuclides in the problem should be very close to 1.

All of these conditions are met for the sensitivity coefficients shown in Table 11.1. Checks 2 and 3 may not be exact if reactions such as (n,3n) are present, because (n,3n) would be included in the scattering sensitivity. Also, there may be small inconsistencies in the cross sections. The reason $\bar{\nu}$ sensitivities do not sum to exactly 1 is discussed in Sect. 3.1.

Sensitivity coefficients can also be checked by making a change in the system and performing a separate transport calculation to calculate the effect of the change directly. A change that is easy to make is to change the number density of an isotope. The sensitivity coefficient for changing a number density is the same as the energy-integrated total cross-section sensitivity coefficient. Changing the number density tests a number of things since the scattering, capture, and fission sensitivities are used to calculate the total sensitivity and $\bar{\nu}$ sensitivities are used to calculate fission sensitivities.

A number of cases where a number density in the base case described above were changed have been analyzed, and the values of k_{eff} for these cases are shown in Table 11.2. A good way to calculate a sensitivity directly is to increase the number density by a certain percentage and also to decrease the number density by the same percentage. A central difference calculation using these two points gives a good approximation for the sensitivity of the base case. Using the values of k_{eff} from Table 11.2 for the 4% changes in the ^{235}U number density, the total cross-section sensitivity for ^{235}U is found to be

$$S_{total} = S_N = \frac{\frac{\Delta k}{k}}{\frac{\Delta N}{N}} = \frac{\frac{1.01462 - 0.994282}{1.00475}}{0.08} = 0.2530 ,$$

and the LAKE-calculated value from Table 11.1 is 0.2529. This agreement is excellent.

A different situation exists when the hydrogen number density is changed by 4%. The sensitivity coefficient obtained by direct calculation is 0.2228; however, the value from LAKE is 0.2890. The reason for this difference is that the direct method is using different resonance-shielded cross sections when the number density is changed. LAKE, on the other hand, is calculating the change caused by changing the number density while using the same cross sections as the base case. When the base-case cross sections are used in a direct calculation, a sensitivity coefficient of 0.2892 is obtained. Again the agreement with the LAKE result is excellent. The difference between the two direct calculations is that changing the hydrogen number density changes the shielded cross sections for ^{238}U, and this effect is not included in the sensitivity formulation.

Table 11.1 Energy-integrated sensitivities for the verification case

ZA	Reaction		Sensitivity
1001	^{1}H	Total	2.8898E-01
1001	^{1}H	Scatter	3.9043E-01
1001	^{1}H	Elastic	3.9041E-01
1001	^{1}H	Capture	-1.0145E-01
1001	^{1}H	n,γ	-1.0145E-01
6012	^{12}C	Total	3.1976E-02
6012	^{12}C	Scatter	3.2646E-02
6012	^{12}C	Elastic	3.2397E-02
6012	^{12}C	n,n’	2.4835E-04
6012	^{12}C	Capture	-6.6977E-04
6012	^{12}C	n,γ	-4.9805E-04
6012	^{12}C	n,p	-3.1008E-08
6012	^{12}C	n,d	-7.8401E-08
6012	^{12}C	n,α	-1.7162E-04
9019	^{19}F	Total	4.7891E-02
9019	^{19}F	Scatter	5.3401E-02
9019	^{19}F	Elastic	3.7476E-02
9019	^{19}F	n,n’	1.5918E-02
9019	^{19}F	n,2n	3.2839E-06
9019	^{19}F	Capture	-5.5107E-03
9019	^{19}F	n,γ	-2.3313E-03
9019	^{19}F	n,p	-2.1735E-04
9019	^{19}F	n,d	-1.0609E-05
9019	^{19}F	n,t	-2.3346E-06
9019	^{19}F	n,α	-2.9491E-03
92235	^{235}U	Total	2.5291E-01
92235	^{235}U	Scatter	4.5200E-04
92235	^{235}U	Elastic	2.8675E-04
92235	^{235}U	n,n’	1.5703E-04
92235	^{235}U	n,2n	1.1003E-05
92235	^{235}U	Fission	3.6453E-01
92235	^{235}U	Capture	-1.1207E-01
92235	^{235}U	n,γ	-1.1207E-01
92235	^{235}U	$\overline{\nu}$	9.4964E-01
92235	^{235}U	χ	9.4964E-01
92238	^{238}U	Total	-2.8689E-01
92238	^{238}U	Scatter	2.7818E-02
92238	^{238}U	Elastic	1.4250E-02
92238	^{238}U	n,n’	1.2534E-02
92238	^{238}U	n,2n	1.0144E-03
92238	^{238}U	Fission	3.3702E-02
92238	^{238}U	Capture	-3.4841E-01
92238	^{238}U	n,γ	-3.4841E-01
92238	^{238}U	$\overline{\nu}$	5.0411E-02
92238	^{238}U	χ	5.0411E-02

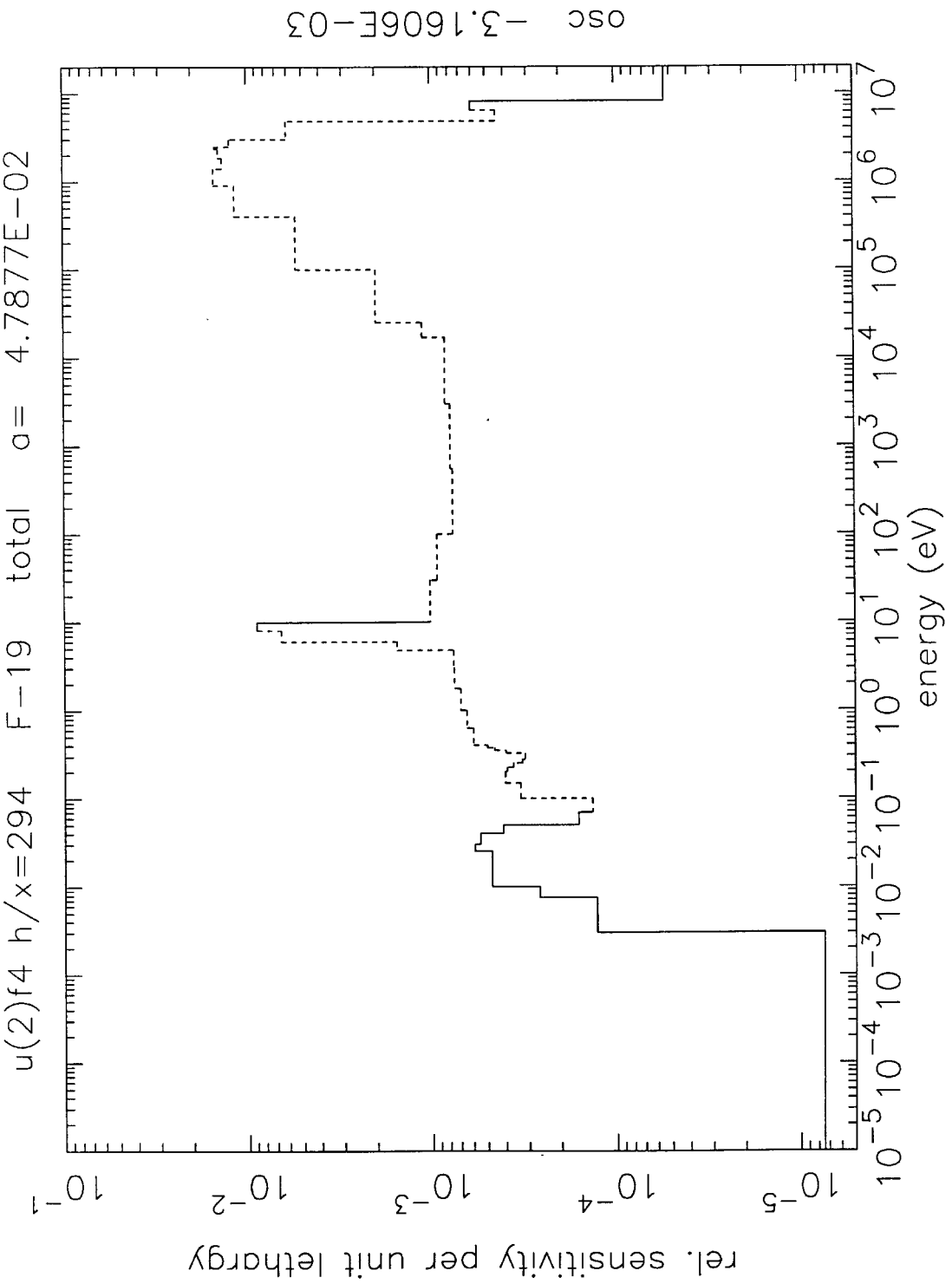


Figure 11.1 ^{19}F total cross-section sensitivity coefficient

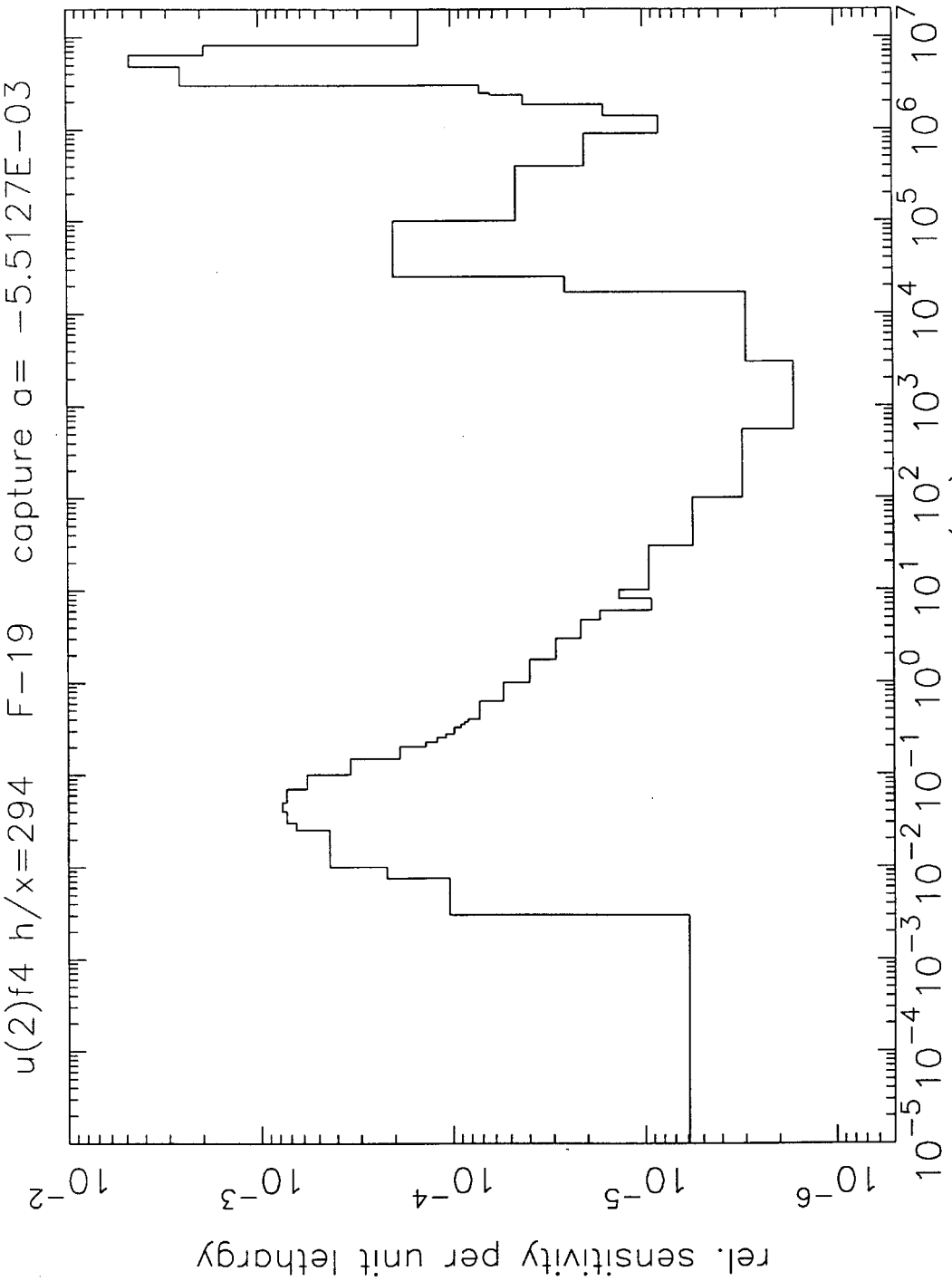


Figure 11.2 ^{19}F capture cross-section sensitivity coefficient

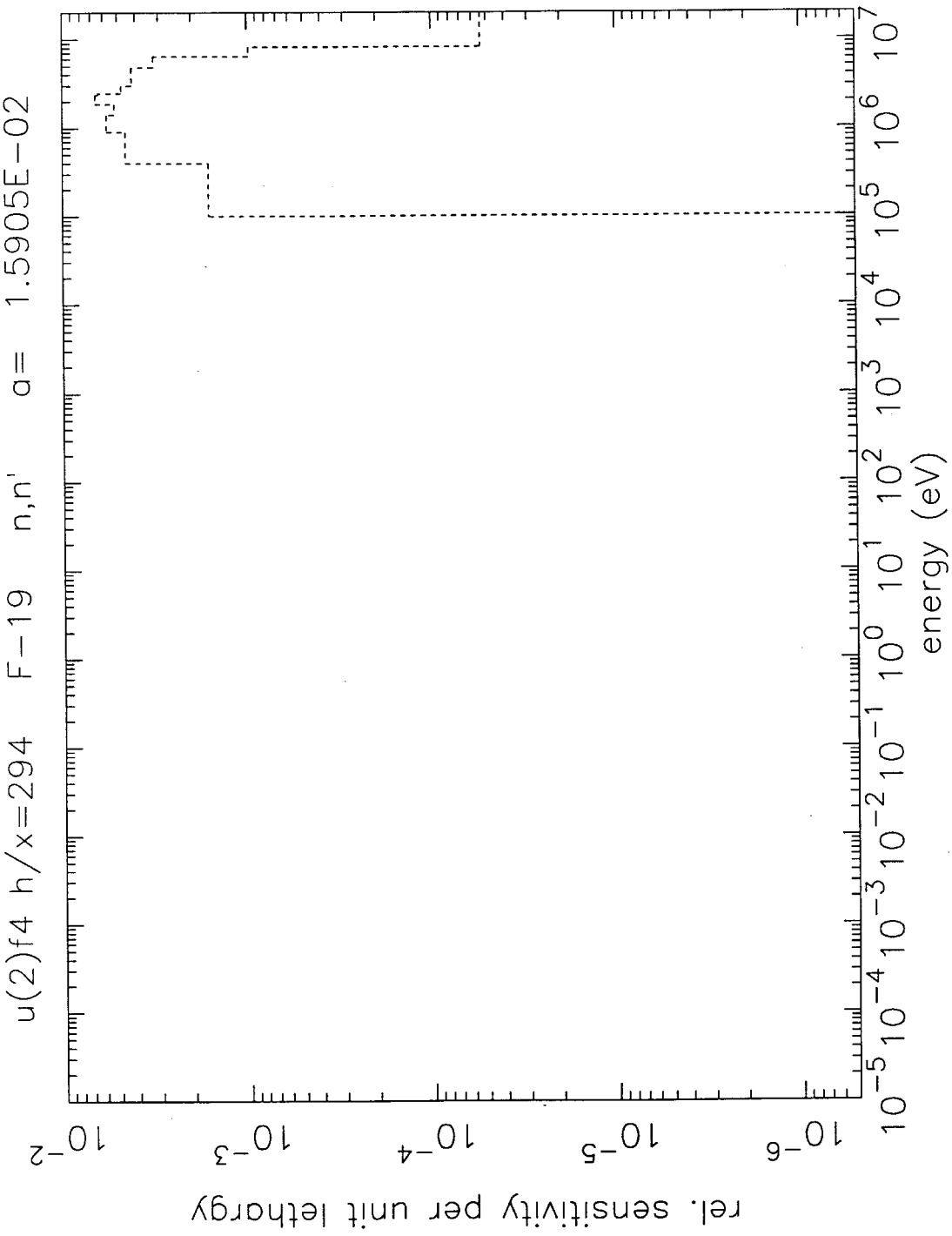


Figure 11.3 ^{19}F (n,n′) cross-section sensitivity coefficient

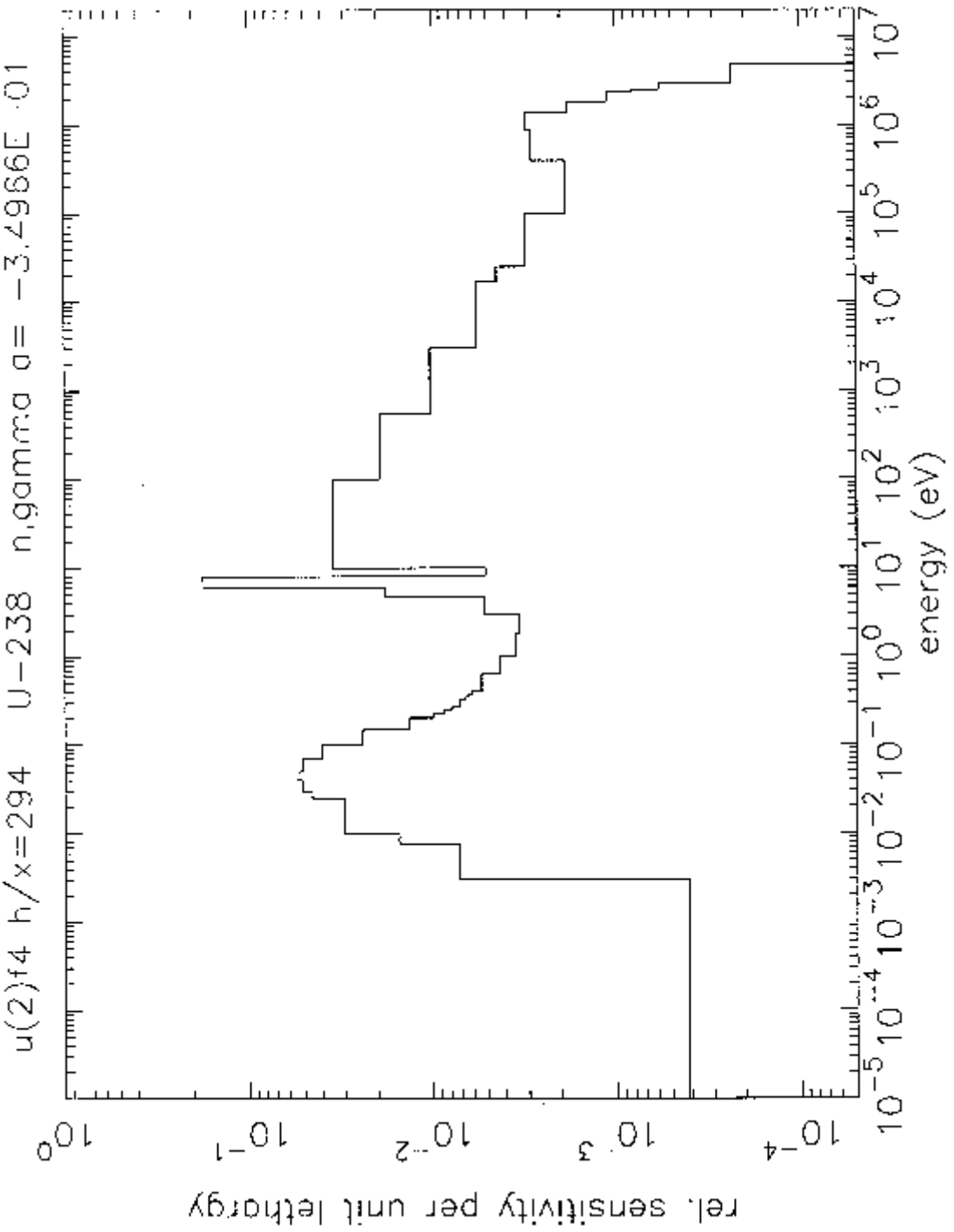


Figure 11.4 ^{238}U (n,() cross-section sensitivity coefficient

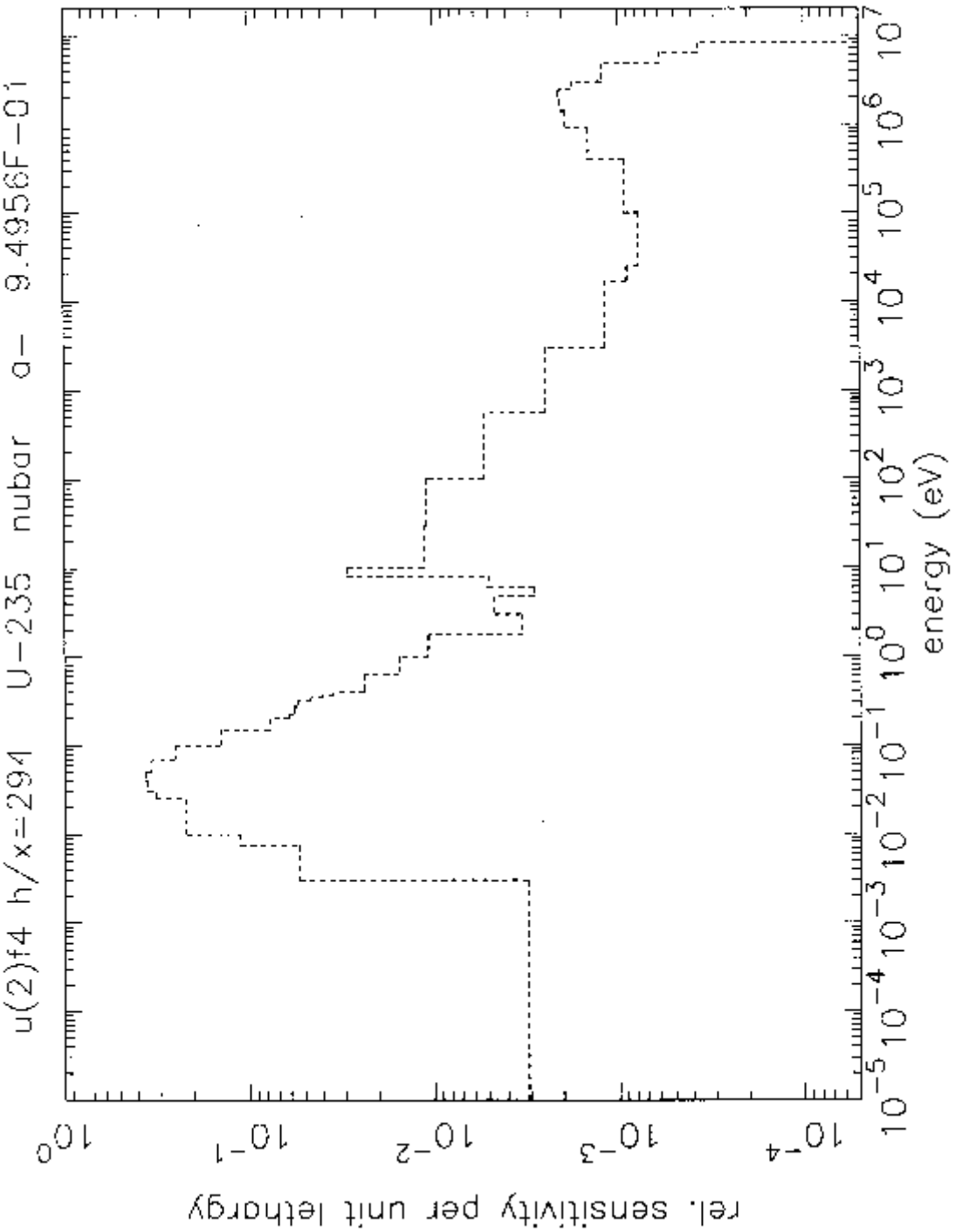


Figure 11.5 ^{235}U Γ cross-section sensitivity coefficient

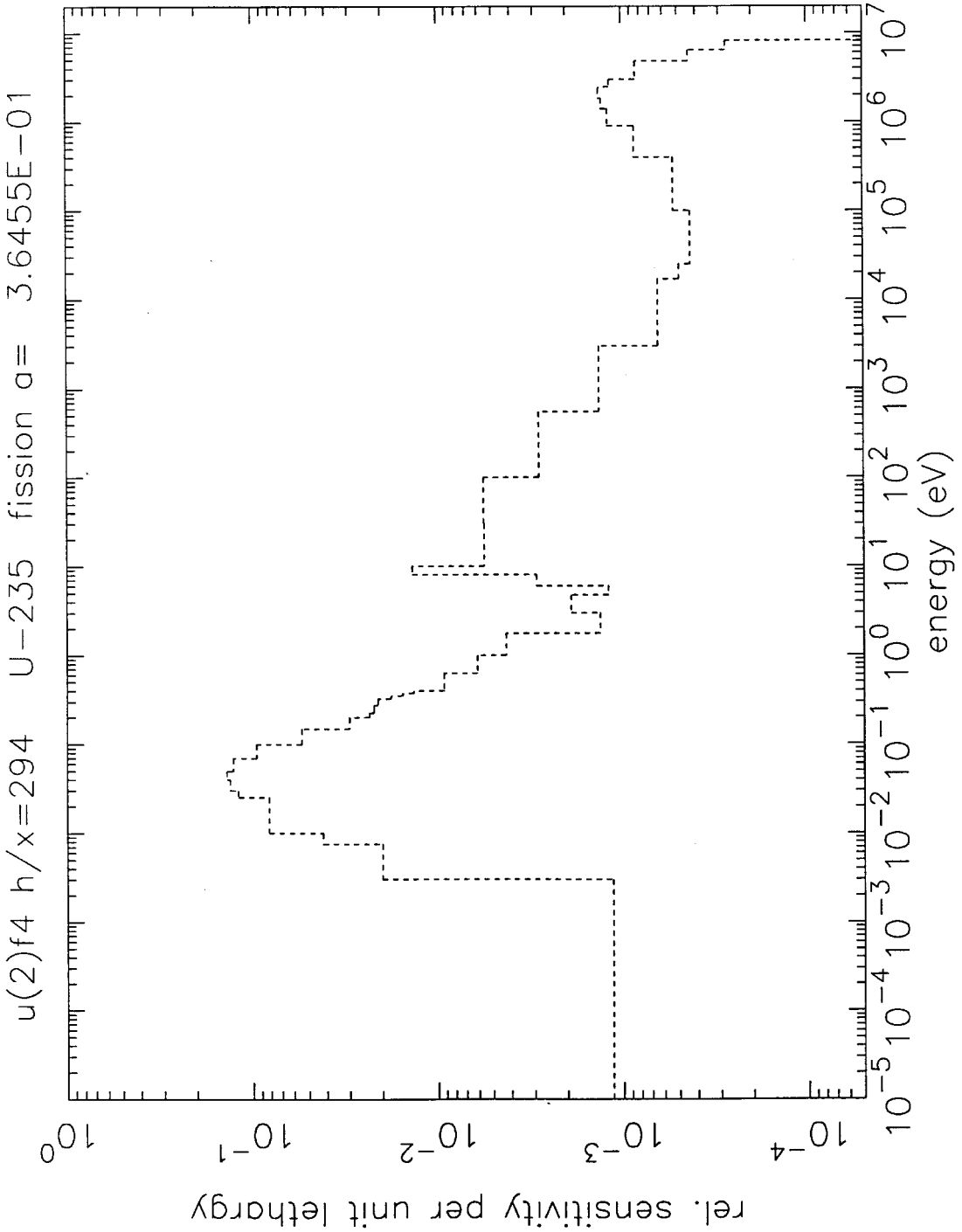


Figure 11.6 ^{235}U fission cross-section sensitivity coefficient

Table 11.2 Calculated values of k_{eff}

Case	k_{eff}
Base case	1.00475
^{235}U atom density decreased 4%	0.994282
^{235}U atom density increased 4%	1.01462
H atom density decreased 4%	0.995401
H atom density decreased 4% (base cross sections)	0.992664
H atom density increased 4%	1.01331
H atom density increased 4% (base cross sections)	1.01591

12 REFERENCES

1. *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluations,* NUREG/CR-0200, Rev. 5 (ORNL/NUREG/CSD-2/R5), Vols. I–III, March 1997. Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-545.

2. C. R. Weisbin, E. M. Oblow, J. H. Marable, R. W. Peelle, and J. L. Lucius, "Application of Sensitivity and Uncertainty Methodology to Fast Reactor Integral Experiment Analysis," *Nucl. Sci. Eng.* **66,** 307–333 (1978).

3. J. L. Lucius et al., *A Users Manual for the FORSS Sensitivity and Uncertainty Analysis Code System,* ORNL-5316, Union Carbide Corp., Oak Ridge Natl. Lab., January 1981.

4. W. A. Rhoades and R. L. Childs, "The DORT Two-Dimensional Discrete Ordinates Transport Code," *Nucl. Sci. Eng.* **99**, 88–89 (May 1988).

5. Cross Section Evaluation Working Group Benchmark Specification, BNL 19302 (ENDF-202), Brookhaven National Laboratory, November 1974.

APPENDIX A

SEN2 TWO-DIMENSIONAL SENSITIVITY ANALYSIS

APPENDIX A

SEN2 TWO-DIMENSIONAL SENSITIVITY ANALYSIS

A.1 TWO-DIMENSIONAL SENSITIVITY ANALYSIS USING DORT

The SCALE sensitivity control sequence SEN1 is used to perform one-dimensional (1-D) sensitivity and uncertainty analyses. This appendix describes how to perform two-dimensional (2-D) sensitivity and uncertainty analyses using the 2-D discrete-ordinates transport code DORT. The objective is to have the same functionality in both 1-D and 2-D, with the main difference being that XSDRNPM is used to obtain forward and adjoint solutions in the 1-D case, while DORT is used in the 2-D case.

The 2-D work has not been made into an automated SCALE sequence because of the following considerations:

1. DORT calculations require much more computer time than XSDRNPM calculations.

2. The DORT geometry and mesh input are more difficult to prepare than the corresponding 1-D input and should be checked before a long calculation is started.

3. DORT calculations sometimes fail to converge adequately and need to be restarted or the input modified to obtain good convergence for the calculated value of k_{eff} and the fluxes.

4. DORT is not a part of the SCALE system.

The first step in performing a 2-D sensitivity/uncertainty analysis is the preparation of problem-dependent cross sections. In SEN1, two cross-section files are used. An AMPX working library is used by XSDRNPM and the LAKE code that performs the sensitivity/uncertainty calculations. Also, a sensitivity cross-section library is used by LAKE. The LAKE code is used for both 1-D and 2-D sensitivity/uncertainty analyses. Thus, the two cross-section files used in SEN1 are also required in nine 2-D analyses. In addition to these two cross-section files, two additional cross-section files are needed: a GIP cross-section file for the forward DORT calculation and a GIP file for the adjoint DORT calculation. A SCALE-type control sequence, SEN2, has been developed to produce all four of the cross-section files needed for 2-D sensitivity analysis. The program description and input description for SEN2 are found in Sect. A.2 of this Appendix.

The second step in performing 2-D sensitivity/uncertainty analyses is to perform both a forward and an adjoint DORT criticality calculation. Two interface files are saved from the forward calculation, and one interface file is saved from the adjoint calculation. A discussion of several topics related to the DORT calculations is found in Sect. A.3 of this Appendix.

The third step in performing 2-D sensitivity/uncertainty analyses is to run the code VIP2D. In the SEN1 sequence, VIP1D reads interface files written by XSDRNPM and writes a file to be read by the LAKE code. Similarly, VIP2D reads the interface files written by DORT (and some other files and input data) and writes a file to be read by the LAKE code. The program description and the input description for VIP2D are found in Sect. A.4 of this Appendix.

The final step in performing 2-D sensitivity/uncertainty analyses is to run the code LAKE. LAKE is also run as part of the SEN1 sequence and is described in Sect. 7 of this report.

Calculations of the Sheba 2 facility at Los Alamos were used to test the sensitivity results obtained using the 2-D sensitivity/uncertainty procedure described above. Figure A.1.1 shows the geometry used for Sheba 2. These results are found in Sect. A.5 of this Appendix.

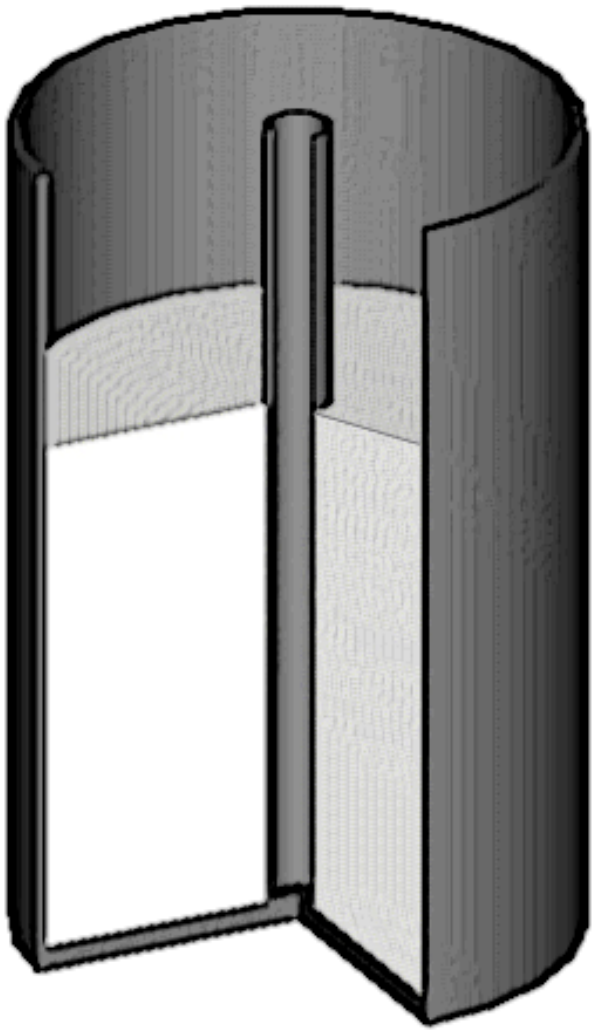


Figure A.1.1 The R-Z geometric model for Sheba 2

A.2 THE SEN2 CROSS-SECTION PROCESSING SEQUENCE

SEN2 is a SCALE-type sequence that prepares the four cross-section files needed for 2-D sensitivity/uncertainty analysis. It also writes a formatted file (fort.30) containing the cross-section mixing table for the problem and other information needed by VIP2D or for preparing the DORT input.

SEN2 was developed by modifying the main program of SEN1. The SEN1 program description is found in Section 5 of this report. None of the subroutines from SEN1 are used in SEN2. Some subroutines from the SCALE subroutine library and MIPLIB are used. One new subroutine, ALPOGIP, was written. ALPOGIP prepares input for ALPO and GIP and writes fort.30. ALPO is an AMPX module available in SCALE that produces an ANISN library from an AMPX working library. GIP is an auxiliary code used with DORT that mixes cross sections from an ANISN library and writes a GIP cross-section file for use by DORT.

The input for SEN2 is very similar to the input for SEN1, described in Sect. 9. The first line of input to SEN2 is the analytical sequence specification record. The analytical sequence specification begins in column 1 of the first line of the input file and must contain either

=SEN2	when INFHOMMEDIUM or MULTIREGION (no cell-weighting) is specified for the type of calculation in the material input processor data to follow, or
=SEN2X	when MULTIREGION or LATTICECELL is specified for the type of calculation in the material input processor data in order to obtain cell-weighted cross sections.

The following optional keyword input may be entered, starting after column 10 of the analytical sequence specification record:

PARM=CHECK PARM=CHK	This option causes the input data to be read and checked without executing any functional modules.
PARM=SIZE=n	The amount of memory requested in four-byte words may be set with this entry. The default value for n is 1000000.
PARM=(CHECK,SIZE=n)	allows checking and size specification.

The next portion of input is the Material Input Processor data. The Material Input Processor data are exactly the same as that used in CSAS, SAS1, SEN1, and other SCALE control modules. Detailed descriptions of this input are found in Sect. C4.4 of the SCALE document.

The final two lines of input to SEN2 are a line containing an integer that specifies the order of scattering expansion for the GIP cross-section libraries and a line with "END" in column 1.

The order of scattering expansion should be at least three since the order of expansion controls the number of flux moments used in the DORT calculations. The flux moments are used to evaluate one of the terms used to calculate the sensitivity coefficients, and a P_1 expansion is not adequate to evaluate this term. Even when a P_1 expansion is adequate to obtain an accurate value for k_{eff}, the DORT calculations still need to use P_3 or higher.

Examples of input for SEN2 are shown in Figures A.2.1 and A.2.2. Notice that SEN2X is specified to obtain cell-weighted cross sections.

The SCALE modules or codes executed by SEN2 are:

BONAMI and NITAWL	To obtain problem-dependent cross sections
XSDRNPM	Called only for SEN2X to provide cell-weighted cross sections
ALPO	To produce an ANISN microscopic cross-section file from the AMPX working library
GIP	To produce a forward GIP macroscopic cross file using the ANISN cross-section file
GIP	To produce an adjoint GIP macroscopic cross file using the ANISN cross-section file

The two unformatted cross-section files produced by SEN2 that are needed by the computer code LAKE to calculate sensitivities are:

1. An AMPX working library. The filename for this library is ft04f001 when SEN2 is used and ft03f001 when SEN2X is used.

2. A sensitivity cross-section library written by NITAWL. The filename for this library is ft20f001.

The unformatted cross-section file needed by the forward DORT case and by VIP2D is the forward GIP cross-section file. The filename for this file is fort.8.

The unformatted cross-section file needed by the adjoint DORT case is the adjoint GIP cross-section file. The filename for this file is fort.18.

The input for the two GIP cases used to generate fort.8 and fort.18 is written by SEN2 in two formatted files named gipf.inp and gipa.inp, respectively. The filename for the unformatted ANISN cross-section library is fort.9. An alternative to saving fort.8 and fort.18 is to save gipf.inp, gipa.inp, and fort.9 and then run GIP to generate fort.8 and fort.18 when they are needed.

Figure A.2.3 shows the contents of the formatted file fort.30 generated by SEN2 for the case shown in Figure A.2.2. This file is read by VIP2D and also contains information needed to prepare the DORT cases. The first line is the title, followed by 10 lines containing values for 10 integer variables. The last lines of the file contain the cross-section mixing table generated by SEN2. Notice that the input for the SEN2 case specifies four mixtures; fort.30 indicates that there are five materials on the GIP library, and the mixing table specifies how to mix mixtures 1 through 5. Mixtures 1 through 4 are the mixtures specified in the SEN2 input, and mixture 5 is the cell-weighted cross-section mixture. In SEN1, the cell-weighted cross section is mixture 500 but that convention is not used with DORT. As in SEN1, mixtures 1 through 3 have been cell-weighted and should not be used in a DORT zone even though they are present on the GIP cross-section file.

Figure A.2.4 shows the contents of the formatted file fort.30 generated by SEN2 for the Sheba 2 case shown in Figure A.2.1.

```
=sen2
sheba ii, 44-grp cross sections
44gr multiregion
u-238  1 0 2.499-3  296. end
u-235  1 0 1.319-4  296. end
u-234  1 0 6.845-7  296. end
u-236  1 0 1.316-6  296. end
o      1 0 3.210-2  296. end
f      1 0 5.334-3  296. end
h      1 0 5.354-2  296. end
ss304  2 1. 296. end
end comp
cylindrical  end
1  23.9
2  25.4
end zone
3
end
```

Figure A.2.1 An example SEN2 input for Sheba 2

```
=sen2x
U(10)O2 p=.7 2-D  leu-comp-therm-032  case 1
44groupndf5                  latticecell
u-234          1  0.0 1.7636e-5 293 end
u-235          1  0.0 2.1577e-3 293 end
u-236          1  0.0 1.53e-5 293 end
u-238          1  0.0 1.951e-2 293 end
o              1  0.0 4.4661e-2 293 end
fe             2  0.0 5.8894e-2 293 end
cr             2  0.0 1.6469e-2 293 end
ni             2  0.0 8.1061e-3 293 end
si             2  0.0 1.3551e-3 293 end
mn             2  0.0 1.299e-3 293 end
c              2  0.0 2.3766e-4 293 end
ti             2  0.0 4.4713e-4 293 end
h2o            3  1.0 293 end
h2o            4  1.0 293 end
end comp
triangpitch .7 .416 1  3  .51 2  .43 0  end
3
end
```

Figure A.2.2 An example SEN2 input with cell-weighting

```
u(10)o2 p=.7 1-d  leu-comp-therm-032  case 1
    3 / isct order of scattering expansion
   44 / igm  no. of groups
    5 / iht  sigma(t) position
   27 / ihs  sigma(g--g) position
   70 / ihm  table length
    5 / mtp  no. of materials from lib. tape
   23 / iftg  first thermal group
   44 / nneut  number of neutron groups
    3 / nt1  unit number for ampx working library
   30 / ms   mixing table length
 mixing table mixture number
             1             5             1             5             1
             5             1             5             1             5
             3             5             4             2             5
             2             5             2             5             2
             5             2             5             2             5
             2             5             3             5             4
 mixing table component
       1092234       1092234       1092235       1092235       1092236
       1092236       1092238       1092238       1008016       1008016
       3008016       3008016       4008016       2026000       2026000
       2024000       2024000       2028000       2028000       2014000
       2014000       2025055       2025055       2006012       2006012
       2022000       2022000       3001001       3001001       4001001
 mixing table number density
  1.763600e-05  5.648719e-06  2.157700e-03  6.911001e-04  1.530000e-05
  4.900510e-06  1.951000e-02  6.248951e-03  4.466100e-02  1.430469e-02
  3.338460e-02  1.731335e-02  3.338460e-02  5.889400e-02  8.196944e-03
  1.646900e-02  2.292177e-03  8.106100e-03  1.128218e-03  1.355100e-03
  1.886046e-04  1.299000e-03  1.807965e-04  2.376600e-04  3.307783e-05
  4.471300e-04  6.223215e-05  6.676920e-02  3.462670e-02  6.676920e-02
```

Figure A.2.3 An example of the contents of file fort.30

```
sheba ii, 44-grp cross sections
    3 / isct order of scattering expansion
   44 / igm  no. of groups
    5 / iht  sigma(t) position
   27 / ihs  sigma(g--g) position
   70 / ihm  table length
    2 / mtp  no. of materials from lib. tape
   23 / iftg  first thermal group
   44 / nneut  number of neutron groups
    4 / nt1  unit number for ampx working library
   14 / ms   mixing table length
 mixing table mixture number
             1             1             1             1             1
             1             1             2             2             2
             2             2             2             2
 mixing table component
       1092238       1092235       1092234       1092236       1008016
       1009019       1001001       2006012       2014000       2015031
       2024304       2025055       2026304       2028304
 mixing table number density
  2.499000e-03  1.319000e-04  6.845000e-07  1.316000e-06  3.210000e-02
  5.334000e-03  5.354000e-02  3.187718e-04  1.702519e-03  6.946803e-05
  1.747259e-02  1.740714e-03  5.854455e-02  7.740198e-03
```

Figure A.2.4 The contents of file fort.30 for the Sheba 2 case

A.3 INPUT CONSIDERATIONS FOR THE DORT CASES

In order to perform a sensitivity/uncertainty analysis using the 2-D transport code DORT, both a forward and an adjoint criticality calculation are required. The input for these two cases must be prepared by the user. The purpose of this section is to give an example of the input for a typical DORT criticality calculation that can be used as a guide to preparing DORT input for criticality calculations.

The input file used for the forward DORT calculation of Sheba 2 is shown in Figure A.3.1. The first line of the file is the title card for the case. This title is not used later for sensitivity plots.

Except for the title card, all of the DORT input file uses FIDO input and must be lowercase. Any information on a line after a "/" is a comment. In the sample input, comments are used in the 61$$, 62$$, and 63** arrays to indicate the name of the input variables being input and to provide a brief description of the function of the variable. Lines that contain "1s" indicate that the input variable is not entered (skipped). In this case, the variable retains its default value if it has 1 or zero if it does not. DORT is distributed by the Radiation Safety Information Computing Center at ORNL as part of the DOORS package (Computer Code Collection Package 650). Documentation for DORT is provided with this package and can be used to learn more about preparing DORT input.

The first FIDO data block contains the 61$$, 62$$, and 63** arrays. In the sample input, values are entered for four of the entries in the 61$$ array. The value on "ntfog" is set to 11 in the forward case and 21 in the adjoint case, causing unformatted flux output files to be written with filenames fort.11 and fort.21. These files are read by the VIP2D code, which is described in the next section. The value of "ntsig" is 8 in the forward case and 18 in the adjoint case, which causes the GIP cross sections to be read from the unformatted files fort.8 and fort.18 respectively. These files were written by SEN2, as described in the previous section. The value of "ntscl" is set to 12 in the forward case and is set to 0 for the adjoint case. This setting results in DORT unformatted scalar flux output file to be written on unit fort.12. To summarize the information entered in the 61$$ array, the forward and adjoint DORT cases read cross sections from files fort.8 and fort.18 and write output files fort.11, fort.12, and fort.21. These three output files must be saved for input to VIP2D.

Thirty values are entered in the 62$$ array of the sample input for Sheba 2. The values of eight of these entries were found in the file fort.30 written by SEN2 and shown in Figure A.2.4. DORT ordinarily allows the user to input a mixing table by entering a value for "mixl" (10th entry in the 62$$ array). For sensitivity work, it is required that all mixture descriptions be specified in the SEN2 input and that no mixing be done in the DORT case.

The number of materials from the cross-section tape is specified using the variable "mtp" (12th entry in the 62$$ array). The value of "mtp" can be found in the file fort.30. The cross-section file for the sample problem contains two materials as specified in the SEN2 input. Originally DORT required that each component of the Legendre expansion be counted as a material such that the number of materials would be entered as 8 for a P_3 cross-section expansion or 12 for a P_5 expansion for the sample problem. Later releases of DORT allow the user to enter the number of physical materials if the mixing table is not used. This option is specified by using the variable "isctc" (70^{th} entry in the 62$$ array) to specify the order of expansion of the GIP cross-section file. The order of Legendre expansion used in the transport calculation is specified by the variable "isctm" (second entry in the 62$$ array). In the sample problem, each of these variables has a value of 3. Use of this feature allows the mixture numbers defined in the SEN2 input to be used in the DORT input without renumbering. In the DORT input, the mixture number by zone is specified in the 9$$ array found near the end of the DORT input file. The total number of materials in the problem is specified using the variable "mtm" (12^{th} entry in the

```
sheba 2
61$$
0            / ntflx    flux guess input unit           if.gt.0
11           / ntfog    flux output unit                if.gt.0
8            / ntsig    cross section unit (default=8)
          1s / ntbsi    boundary source input unit      if.gt.0
          1s / ntdsi    distributed source input unit   if.gt.0 (must supply scratc
             /  5
          1s / ntfci    reserved (enter 0)
          1s / ntibi    internal boundary source input  if.gt.0
          1s / ntibo    internal boundary flux output   if.gt.0
          1s / ntnpr    large-scale print unit          if.gt.0
          1s / ntdir    directional flux output unit    if.gt.0
             / 10
          1s / ntdso    distributed source output unit  if.gt.0
12           / ntscl    scalar flux output unit         if.gt.0
          1s / ntznf    zone   flux output unit         if.gt.0
  e
62$$
0            / iadj     0=forward calculation; 1=adjoint
3            / isctm    maximum order of pl scattering
3            / izm      number of material zones
57           / im       number of radial intervals (negative implies variable mesh
126          / jm       number of axial intervals
             /  5
44           / igm      number of energy groups
5            / iht      position of total cross section
27           / ihs      position of self-scatter cross section
70           / ihm      cross section table length per group
          1s / mixl     mixing table length
             / 10
4            / mmesh    number of material zone bodies (0=no effect)
2            / mtp      number of materials from ntsig (0 implies mtm)
3            / mtm      total number of materials
          1s / idfac    0=no density factors; 1=input dens(i,j)
160          / mm       maximum number of directions in quadrature (negative indica
             / 15
1            / ingeom   0=x-y geometry; 1=r-z; 2=r-theta; 3=180-360 triangle; 4=60
1            / ibl      (0=void         4=fxd bndry srce)
0            / ibr      (1=reflected    5=albedo        )
0            / ibb      (2=periodic                     )
          1s / ibt      (3=cylindrical                  )
             / 20
100          / isrmx    source iteration maximum
-20          / ifxmi    initial flux iteration maximum per group          (negativ
          1s / ifxmf    final   flux iteration maximum per group (if.ne.0) (negativ
          1s / mode     0=lin-zero; 1=linear; 2=scalar wtd; 3=0 wtd; 4=theta wtd; 5
```

Figure A.3.1 DORT input for the Sheba 2 forward case

```
1           / ktype    0=fixed source; 1=k search; 2=db2 search; 3=concentration s
            / 25
          1s / iacc    0=groupwise rebalance; 1=diffusion acceleration; 2=partial
          1s / kalf    0=standard acceleration procedure; 1=alternate
          1s / igtype  0=discrete ordinates; n=theory specified by group for n out
3           / inpfxm   0=flux guess 0 or on ntflx; 1=fij(i,j) g times; 2=fij(i,j)*
0           / inpsrm   distributed source input, same as inpfxm (requires ntdsi.gt
            / 30
          1s / njntsr  0=no effect; n=interior boundary source at n j-boundaries i
          1s / nintsr  0=no effect; n=interior boundary source at n i-boundaries i
          1s / njntfx  0=no effect; n=interior boundary flux   at n j-boundaries w
          1s / nintfx  0=no effect; n=interior boundary flux   at n i-boundaries w
0           / iact     0=no effect; n=calculate n activities (negative bypasses po
            / 35
3           / ired     -1=izm regions, system balances only; 0=no bal; 1=1 region;
          1s / ipdb2   0=no effect; 1=punch average db2 value; 2=igm values; 3=igm
          1s / ifxprt  0=scalar flux printed; 1=not printed; 2= printed as calc (+
          1s / icsprt  0=cross sections printed; 1=not printed
          1s / idirf   0=directional flux not saved; 1=saved and printed; 2=saved
            / 40
          1s / jdirf   first axial interval for directional flux output  (0=no eff
          1s / jdirl   last  axial interval for directional flux output  (0=no eff
          1s / nbuf    no effect
          1s / iepsbz  0=no effect; 1=use zone impt convg; 11=use & print final co
          1s / minblk  minimum j-blocking (0=all groups stored in memory if possib
            / 45
1           / maxblk   maximum j-blocking          (0 implies jm)
          1s / isbt    i set for boundaries          (default=1)
          1s / msbt    m set for boundaries          (default=1)
          1s / msdm    m set for dimensioning        (default=1)
          1s / ibfscl  no. flux itns before accel    (default=1)
            / 50
          1s / intscl  min no. flux acceleration itns  (default=4)
          1s / itmscl  max no. flux acceleration itns  (default=50)
          1s / nofis   0=normalized fission; 1=unnormalized; 2=none (default=1)
          1s / ifdb2z  0=no effect; 1=db2 supplied by group, then by region
          1s / iswp    type of diffusion theory sweep  (rv=4 or 5)
            / 55
          1s / keyjn   j-interval for key flux output  (default=1)
          1s / keyin   i-interval for key flux output  (default=1)
          1s / nsigtp  reserved (use 0)
          1s / norpos  c.s. position for normalization (0 ignored)
          1s / normat  c.s. material for normalization (0 indicates macro in each
            / 60
          1s / mstmax  maximum number of m-sets (0 implies mstmx=jm)
0           / negfix   0=none; 1=full source fix up; 2=initial fix up; -1=economy
03500       / locobj   initial memory allocation, words*1000 (0 implies use defaul
          1s / lcmobj  file segment size, words*1000 (0 implies unlimited segment
          1s / nkeyfx  length of key flux array (negative prints array only at gro
            / 65
```

Figure A.3.1 (continued)

```
0            / ncndin   maximum user condition code (default=4)
44           / neut     last neutron group          (default=-1; implies igm)
          1s / itally   0: no effect; -1: internal timing analysis
          1s / neutac   0: no effect; n=activities over first n groups only
3            / isctc    order of cross section expansion (if .gt.0)
  e
63**
          1s / tmax     maximum cpu time for this prob         (0.0=no effect)
1            / xnf      source normalization factor            (0.0=no effect)
5-7          / eps      eigenvalue convergence criterion       (default=1.0e-4)
1-5          / epp      pointwise flux convergence criterion   (default=1.0e-3)
          1s / epv      volumetric flux convergence criterion
             /  5
1-5          / epf      fission convergence criterion          (default=1.0e-3)
          1s / ekobj    keff sought in b, c, d search; k estimate in k search
          1s / evth     keff convergence ratio                 (default=0.2)
          1s / evchm    maximum ev change ratio, each itn      (default=1.5)
          1s / evmax    maximum ev change ratio, overall       (default=10.0)
             / 10
          1s / evkmx    maximum valid keff-ekobj               (default=1.0)
          1s / evi      initial eigenvalue                     (default=1.0)
          1s / devdki   initial eigenvalue slope               (default=-1.0)
          1s / evdelk   initial eigenvalue increment           (default=0.3)
          1s / sormin   maximum source iteration acceleration  (default=10.0)
             / 15
.5           / conacc   flux acceleration acceptance criterion (default=1.)
          1s / conscl   flux acceleration converg.   criterion (default=1.0e-4)
          1s / coneps   flux acceleration convergence ratio    (default=0.01)
          1s / wsolmn   reserved (use 0)
0            / wsolii   flux acceleration damping increment    (neg: use only as re
             / 20
4            / wsolcn   flux acceleration damping constant     (neg: use only on fi
          1s / orf      diffusion theory flux acceleration  parameter (default=0.6)
          1s / fsnacc   reserved (use 0)
          1s / flxmin   minimum flux for convergence tests            (default=1.0e
          1s / smooth   reserved (use 0)
             / 25
1-4          / epo      source iteration flux convergence criterion
          1s / extrcv   extrapolation convergence criterion          (default=0.2)
          1s / theta    theta-weighting parameter                    (default=0.9)
          1s / esp1     reserved (use 0)
          1s / esp2     reserved (use 0)
  e
  t
  t
/  s  16 full symmetric
```

Figure A.3.1 (continued)

```
82*
 0 -21082- 5 0 -14907- 5 0 +14907- 5 0 -42164- 5 0 -39441- 5 0 -14907- 5
 0 +14907- 5 0 +39441- 5 0 -55777- 5 0 -53748- 5 0 -39441- 5 0 -14907- 5
 0 +14907- 5 0 +39441- 5 0 +53748- 5 0 -66667- 5 0 -64979- 5 0 -53748- 5
 0 -39441- 5 0 -14907- 5 0 +14907- 5 0 +39441- 5 0 +53748- 5 0 +64979- 5
 0 -76012- 5 0 -74536- 5 0 -64979- 5 0 -53748- 5 0 -39441- 5 0 -14907- 5
 0 +14907- 5 0 +39441- 5 0 +53748- 5 0 +64979- 5 0 +74536- 5 0 -84327- 5
 0 -82999- 5 0 -74536- 5 0 -64979- 5 0 -53748- 5 0 -39441- 5 0 -14907- 5
 0 +14907- 5 0 +39441- 5 0 +53748- 5 0 +64979- 5 0 +74536- 5 0 +82999- 5
 0 -91894- 5 0 -90676- 5 0 -82999- 5 0 -74536- 5 0 -64979- 5 0 -53748- 5
 0 -39441- 5 0 -14907- 5 0 +14907- 5 0 +39441- 5 0 +53748- 5 0 +64979- 5
 0 +74536- 5 0 +82999- 5 0 +90676- 5 0 -98883- 5 0 -97753- 5 0 -90676- 5
 0 -82999- 5 0 -74536- 5 0 -64979- 5 0 -53748- 5 0 -39441- 5 0 -14907- 5
 0 +14907- 5 0 +39441- 5 0 +53748- 5 0 +64979- 5 0 +74536- 5 0 +82999- 5
 0 +90676- 5 0 +97753- 5 0 -21082- 5 0 -14907- 5 0 +14907- 5 0 -42164- 5
 0 -39441- 5 0 -14907- 5 0 +14907- 5 0 +39441- 5 0 -55777- 5 0 -53748- 5
 0 -39441- 5 0 -14907- 5 0 +14907- 5 0 +39441- 5 0 +53748- 5 0 -66667- 5
 0 -64979- 5 0 -53748- 5 0 -39441- 5 0 -14907- 5 0 +14907- 5 0 +39441- 5
 0 +53748- 5 0 +64979- 5 0 -76012- 5 0 -74536- 5 0 -64979- 5 0 -53748- 5
 0 -39441- 5 0 -14907- 5 0 +14907- 5 0 +39441- 5 0 +53748- 5 0 +64979- 5
 0 +74536- 5 0 -84327- 5 0 -82999- 5 0 -74536- 5 0 -64979- 5 0 -53748- 5
 0 -39441- 5 0 -14907- 5 0 +14907- 5 0 +39441- 5 0 +53748- 5 0 +64979- 5
 0 +74536- 5 0 +82999- 5 0 -91894- 5 0 -90676- 5 0 -82999- 5 0 -74536- 5
 0 -64979- 5 0 -53748- 5 0 -39441- 5 0 -14907- 5 0 +14907- 5 0 +39441- 5
 0 +53748- 5 0 +64979- 5 0 +74536- 5 0 +82999- 5 0 +90676- 5 0 -98883- 5
 0 -97753- 5 0 -90676- 5 0 -82999- 5 0 -74536- 5 0 -64979- 5 0 -53748- 5
 0 -39441- 5 0 -14907- 5 0 +14907- 5 0 +39441- 5 0 +53748- 5 0 +64979- 5
 0 +74536- 5 0 +82999- 5 0 +90676- 5 0 +97753- 5
83*
 3r-97753- 5 5r-90676- 5 7r-82999- 5 9r-74536- 511r-64979- 513r-53748- 5
15r-39441- 517r-14907- 5 3r+97753- 5 5r+90676- 5 7r+82999- 5 9r+74536- 5
11r+64979- 513r+53748- 515r+39441- 517r+14907- 5
81*
 0 +    0+ 0 2r+13586- 6 0 +    0+ 0 0 +97681- 7 2r+97681- 7 0 +97681- 7
 0 +    0+ 0 0 +64738- 7 0 +50390- 7 2r+64738- 7 0 +50390- 7 0 +64738- 7
 0 +    0+ 0 0 +64634- 7 0 +71124- 7 0 +71124- 7 2r+64634- 7 0 +71124- 7
 0 +71124- 7 0 +64634- 7 0 +    0+ 0 0 +64634- 7 0 +14381- 7 0 +36342- 7
 0 +14381- 7 2r+64634- 7 0 +14381- 7 0 +36342- 7 0 +14381- 7 0 +64634- 7
 0 +    0+ 0 0 +64738- 7 0 +71124- 7 0 +36342- 7 0 +36342- 7 0 +71124- 7
 2r+64738- 7 0 +71124- 7 0 +36342- 7 0 +36342- 7 0 +71124- 7 0 +64738- 7
 0 +    0+ 0 0 +97681- 7 0 +50390- 7 0 +71124- 7 0 +14381- 7 0 +71124- 7
 0 +50390- 7 2r+97681- 7 0 +50390- 7 0 +71124- 7 0 +14381- 7 0 +71124- 7
 0 +50390- 7 0 +97681- 7 0 +    0+ 0 0 +13586- 6 0 +97681- 7 0 +64738- 7
 0 +64634- 7 0 +64634- 7 0 +64738- 7 0 +97681- 7 2r+13586- 6 0 +97681- 7
 0 +64738- 7 0 +64634- 7 0 +64634- 7 0 +64738- 7 0 +97681- 7 0 +13586- 6
 0 +    0+ 0 2r+13586- 6 0 +    0+ 0 0 +97681- 7 2r+97681- 7 0 +97681- 7
 0 +    0+ 0 0 +64738- 7 0 +50390- 7 2r+64738- 7 0 +50390- 7 0 +64738- 7
 0 +    0+ 0 0 +64634- 7 0 +71124- 7 0 +71124- 7 2r+64634- 7 0 +71124- 7
```

Figure A.3.1 (continued)

```
 0 +71124- 7 0 +64634- 7 0 +    0+ 0 0 +64634- 7 0 +14381- 7 0 +36342- 7
  0 +14381- 7 2r+64634- 7 0 +14381- 7 0 +36342- 7 0 +14381- 7 0 +64634- 7
  0 +    0+ 0 0 +64738- 7 0 +71124- 7 0 +36342- 7 0 +36342- 7 0 +71124- 7
  2r+64738- 7 0 +71124- 7 0 +36342- 7 0 +36342- 7 0 +71124- 7 0 +64738- 7
  0 +    0+ 0 0 +97681- 7 0 +50390- 7 0 +71124- 7 0 +14381- 7 0 +71124- 7
  0 +50390- 7 2r+97681- 7 0 +50390- 7 0 +71124- 7 0 +14381- 7 0 +71124- 7
  0 +50390- 7 0 +97681- 7 0 +    0+ 0 0 +13586- 6 0 +97681- 7 0 +64738- 7
  0 +64634- 7 0 +64634- 7 0 +64738- 7 0 +97681- 7 2r+13586- 6 0 +97681- 7
  0 +64738- 7 0 +64634- 7 0 +64634- 7 0 +64738- 7 0 +97681- 7 0 +13586- 6
   t
 1**
   4.992653-03  1.387983-02  4.373482-02  1.526830-01  8.539175-02
   2.416508-02  1.150210-01  1.268105-01  1.647279-01  1.725747-01
   8.257210-02  1.171736-02  7.566955-04  9.001997-04  6.679648-05
   5.254233-06  3.690851-07  5.860683-08  3.785072-09  3.690678-09
   1.918879-09  2.277392-09  1.254941-09  5.983969-10  2.234389-10
   1.064994-10  1.030954-11  9.971495-12  9.621686-12  1.813864-11
   8.485238-12  8.070835-12  7.634051-12  1.384570-11  1.169212-11
   5.787015-12  3.241903-12  1.404690-12  1.238359-12  5.176227-13
   1.335696-12  1.547977-13  2.143079-13  7.256248-14
 2** 4i-2.54 86i0 29i43.5 3i73.7 75.605
 4** 3i0 1i2.36 47i3 2i23.9 25.4
 9$$ 1 2 3
28$$ f1
31$$ 2 1 3 3
32** 0 3 0 3
33** 25.4 23.9 2.36 23.9
34** -2.54 0 -2.54 43.5
35** 75.605 73.7 75.605 73.7
t
93** f1
t
94** f1
t
95** 1 f0
  t
```

Figure A.3.1 (continued)

62$$ array). In the sample problem, the total number of materials in the problem is three. The first two materials are from the GIP file, and material 3 is a void. In DORT a void must not be specified as material 0 as is done in SEN1 or XSDRNPM.

The sixth through ninth entries of the 62$$ array contain four entries that describe the cross-section tables on the GIP cross-section file. The values for these variable can be taken from fort.30.

The 11th entry of the 62$$ array specifies that material zone bodies are used to describe the geometry. Other methods of geometry input are allowed in DORT, and the user may use these methods if desired.

The 14th entry of the 62$$ array is used to specify density factors. For sensitivity calculations, density factors must not be used since cross-section specifications must be done in the SEN2 input only.

The 15th entry of the 62$$ array specifies the number of directions in the discrete-ordinates quadrature set. For the sample problem, the number of directions is 160, which corresponds to an S16 quadrature. DORT requires that quadrature sets contain zero-weight angles. For criticality sensitivity studies, the quadratures supplied with the DORT distribution are probably sufficient. DORT input requires that the quadrature input be included in the input file. This step is done by copying the 81*, 82*, and 83* arrays from the file supplied with DORT to the input file.

The 16th through 20th entries of the 62$$ array specify the type of geometry and boundary conditions used in the discrete-ordinates calculation. The geometry can be X-Y, R-Z, or R-θ. Any of the boundary conditions allowed by DORT, except boundary sources, may be used. No external sources are allowed in criticality calculations.

Entries 21 and 22 of the 62$$ array specify the maximum number of source and flux iterations for the problem. The number of source (or outer) iterations for the sample problem is 100. In the sample problem, the maximum number of flux (or inner) iterations per group is entered as a negative number, which indicates that this information is entered by group in the 28$$ array. For the sample problem, the 28$$ array is filled with the value 1 such that one inner iteration per group is performed for each outer iteration. The sample problem (forward case) was also run using two inners per group to see how much CPU time was required. On a Decstation 500 workstation, the one-inner-per-outer case took 71 outer iterations and 56.6 minutes of CPU while the two-inners-per-outer case took 63 outer iterations and 84.1 minutes of CPU. Thus, for this problem, the one-inner-per-outer case requires significantly less CPU time. The 44-group SCALE library used for this case has 22 thermal groups with upscatter. DORT has relatively little upscatter acceleration (mainly fission error mode extrapolation of the fission source and fluxes) and thus requires about 70 outer iterations to obtain a very well-converged solution for the Sheba 2 problem. For this example, the two-inners-per-outer case does not reduce the number of outers very much and thus requires considerably more CPU time.

The 24th and 25th entries in the 62$$ array specify the differencing method and type of calculation for the discrete-ordinates calculation. The default value of 4 was used for "mode," indicating that the theta-weighted differencing method be used. *Mode 3 (zero-weighted) should never be used for criticality calculations since it does not give accurate results.* Mode 0 (linear with zero fix up) can be used, but for the sample problem the fluxes do not converge well because of oscillations, while Mode 4 converges smoothly. For criticality calculations, "ktype" must have the value 1.

The default values are used for the 26th through 28th entries of the 62$$ array of the sample problem. These options specify that partial current rebalance and the method of discrete ordinates are used. The diffusion-theory option of DORT should not be used for sensitivity work.

The 29th and 30th entries in the 62$$ array describe the flux guess and source description for the DORT case. A nonzero flux guess must be provided, and the source must be zero for criticality calculations.

The 45th and 46th entries in the 62$$ array determine what portions of the fluxes are stored in memory. The default value of "minblk" is zero, which specifies that all fluxes are to be stored in memory if possible. The maximum amount of memory that DORT will attempt to use is specified by "locobj" (entry 63 in the 62$$ array). The sample problem was run with all fluxes in memory and used 3.5 million words of memory. For problems where all of the fluxes cannot be stored in memory, the user should attempt to store fluxes for one group at a time in memory. This procedure is done by setting "maxblk" to 1.

The variable "negfix" (entry 62 in the 62$$ array) is used to specify whether negative angular sources caused by the Legendre expansion of the scattering cross section should be corrected. For many criticality calculations, this fix-up is not needed. When the linear-zero flux extrapolation model ("mode" = 0) was tested for the sample problem, the use of a negative fix up was required to prevent division by zero. When a negative fix-up is needed, the full source fix-up ("negfix" = 1) is better than the economy fix-up, which does not conserve neutrons and should not be used for criticality calculations.

Eight values are specified in the 63** array of the sample problem. Most of these values are convergence criteria. Entries 20 and 21 of the 63** array are used to turn off the variable damping feature of the partial current inner iteration acceration method for the sample problem. This feature was designed primarily to be used for shielding problems and can result in very large damping factors when many outers are performed.

The error-mode extrapolation is controlled by the variable "extrcv" (27th entry in the 63** array). The default value is used in the sample problem. The value of error-mode extrapolation for the sample problem was tested by setting "extrcv" to zero. Without error-mode extrapolation, 151 outers and 126.5 min of CPU were required to obtain convergence. Recall that 71 outers and 56.6 min were required with error-mode extrapolation.

Notice that there are two FIDO terminators ("t") after the first FIDO data block of the sample problem. This occurs because no data were entered for the second data block, but the terminator is required even when no data are entered. The third data block for the sample problem contains the 81**, 82**, and 83** arrays that are used to enter the angular quadrature.

In the fourth FIDO data block, the user is required to enter a 1** array containing the fission spectrum (χ) for the problem. DORT allows only one fission spectrum for the entire problem. In contrast, XSDRNPM uses a different fission spectrum for each material, and these fission spectra are determined from the data on the AMPX working cross-section library. One way to obtain a fission spectrum for use in DORT is to perform a 1-D sensitivity calculation using SEN1. SEN1 will write an unformatted file with filename "chi" that contains all of the fission spectra used by XSDRNPM in the SEN1 calculation. By choosing a 1-D problem that contains the same material as the most important material in the DORT case, a fission spectrum appropriate to the DORT problem is obtained. The uppercase "E" in the exponents of the fission spectrum must be converted to lowercase or removed for use in DORT.

The flux guess used for the sample problem is flat in space and zero for all groups except the highest-energy group. The important thing to note about this flux guess is that it is zero in all of the thermal groups. If a nonzero flux guess that is much too large is used for the thermal groups, many outer iterations will be required to reduce the thermal flux to its converged value. The danger is that all of the outer iterations allowed for the problem will be used and the thermal flux will still be much too large.

An example of a DORT criticality calculation that can be very hard to converge is the adjoint calculation for a system with a thick water reflector. In this calculation, the importance of neutrons near the outside of the reflector is very low. The adjoint fluxes near the outside of the reflector are difficult to converge even when the forward case converges well. These very low adjoint fluxes (importances) tend to oscillate. For this class of problems, the convergence of the problem should be judged by the convergence of k_{eff} and the fission density. The flux guess for the thermal groups in adjoint problems should be zero.

For the adjoint version of the Sheba 2 case, the following changes were made to the forward case:

ntfog was changed from 11 to 21 (entry 2 of the 61$$ array)
ntsig was changed from 8 to 18 (entry 3 of the 61$$ array)
ntscl was changed from 12 to 0 (entry 12 of the 61$$ array)
iadj was changed from 0 to 1 (entry 1 of the 62$$ array)
The energy dependence of the flux guess was changed by modifying the 95** array input as follows:
"95** 43r0 1."

Note that the energy dependence in the adjoint flux guess is entered in reverse order such that this flux guess is in the last group, which corresponds to the highest-energy group.

A.4 VIP2D INPUT DESCRIPTION

VIP2D is a program that reads the flux files written by forward and adjoint DORT criticality calculations and writes an output file that is read by the program LAKE. LAKE is a program that performs sensitivity and uncertainty analysis. VIP2D has the same role in 2-D sensitivity/uncertainty analysis as VIP1D has in 1-D. VIP1D reads output files written by XSDRNPM; VIP2D reads flux files written by DORT. VIP1D is described in Sect. 6 of this report.

VIP2D requires the following six files as input:

1. the unformatted flux output file written by the forward DORT case on unit "ntfog" (filename is fort.11),

2. the unformatted flux output file written by the adjoint DORT case on unit "ntfog" (filename is fort.21),

3. the unformatted scalar flux output file written by the forward DORT case on unit "ntscl" (filename is fort.12),

4. the unformatted GIP cross-section file written by SEN2 and read by the forward DORT case on unit "ntsig" (filename is fort.8),

5. the formatted file (filename fort.30) written by SEN2, and

6. a formatted input file with filename "input."

The first line of the VIP2D input file is a title card. The first 80 columns of the title card are written on the interface file written by VIP2D and read by LAKE. The first 16 columns of the title card are used to label sensitivity plots.

The second line of the VIP2D input file describes the geometry used in the DORT cases and should contain the value used for the DORT input variable "ingeom" (16th entry in the 62$$ array.) This variable is 0 for X-Y geometry, 1 for R-Z geometry, and 2 for R-θ geometry.

The last information in the VIP2D input file is the 1** array from the DORT cases followed by a "t" FIDO terminator. The 1** array contains the fission spectrum used by DORT.

The VIP2D input file used to analyze the Sheba 2 experiment is shown in Figure A.4.1.

The printed output from VIP2D is very short. It consists of the title card, a few variables describing the DORT calculations, and the values of k_{eff} from the forward and adjoint DORT calculations. This information is also printed by LAKE.

In addition to the short printed output, VIP2D writes an unformatted interface file with filename ft33f001. This file is read by the LAKE code. The description of this file is found in Sect. 6.

The mixing table written on the interface file is obtained from the file fort.30 written by SEN2, as is the length of the mixing table MS.

The array SCAT on the interface file is calculated using the flux moments from DORT, as indicated in Eq. (3.11). The sign of the odd moments of SCAT ($\ell = 1$ and $\ell = 3$ for the P_3 case) is changed to account for the fact that the adjoint fluxes correspond to the importance of neutrons traveling in the reverse direction. This correction was not required in VIP1D because the adjoint angular fluxes were reversed in direction by XSDRNPM.

The array TOTPP on the interface file is calculated using the flux moments, rather than angular fluxes as was done in the 1-D case. The use of flux moments to evaluate this term is the reason that the DORT calculations should be at least P_3 even if a P_1 cross-section expansion is adequate to calculate k_{eff}. In terms of the notation used in Sect. 3, the equation for evaluating T_g is

$$T_g = V \sum_{\ell=0}^{\infty} (2\ell + 1) \sum_{n=0}^{\ell} \phi_{g,\ell,n} \phi^*_{g,\ell,n} \quad .$$

The ℓ and n subscripts indicate that the angular dependence of the forward and adjoint fluxes are represented by spherical harmonic expansions. The summation over ℓ is truncated at the order of expansion used in the DORT problem. Further discussion of the use of flux moments to evaluate perturbation equations can be found in Ref. A.1.

Because the energy-dependent leakage from the DORT case is not easily accessible by VIP2D, the array TLEAKAGE on the interface file is filled with 0.0. This omission does not affect the sensitivity calculation. LAKE does not print the four lines of output that describe the leakage for the 2-D case.

```
sheba 2
1
 1**
  4.992653-03  1.387983-02  4.373482-02  1.526830-01  8.539175-02
  2.416508-02  1.150210-01  1.268105-01  1.647279-01  1.725747-01
  8.257210-02  1.171736-02  7.566955-04  9.001997-04  6.679648-05
  5.254233-06  3.690851-07  5.860683-08  3.785072-09  3.690678-09
  1.918879-09  2.277392-09  1.254941-09  5.983969-10  2.234389-10
  1.064994-10  1.030954-11  9.971495-12  9.621686-12  1.813864-11
  8.485238-12  8.070835-12  7.634051-12  1.384570-11  1.169212-11
  5.787015-12  3.241903-12  1.404690-12  1.238359-12  5.176227-13
  1.335696-12  1.547977-13  2.143079-13  7.256248-14
  t
```

Figure A.4.1 VIP2D input file for the Sheba 2 experiment

A.5 VERIFICATION OF THE TWO-DIMENSIONAL SENSITIVITY CALCULATIONS

Verification of the 1-D sensitivity/uncertainty control sequence SEN1 is presented in Sect. 11 of this report. The purpose of this section is to test the correctness of 2-D sensitivity calculations performed using the SCALE-like sequence SEN2 and the codes DORT, VIP2D, and LAKE. SEN2 and VIP2D are new codes and have not been tested previously. DORT has been in use for many years but has been used primarily for shielding work. LAKE is also used by SEN1 and has been tested in the 1-D work. A number of DORT and KENO V.a calculations have been performed to confirm that SEN2, DORT, VIP2D, and LAKE are working correctly. The critical experiment used for these calculations was Sheba 2. The calculated values of k_{eff} obtained are shown in Table A.5.1.

The values of k_{eff} calculated by DORT were compared with values of k_{eff} from KENO V.a for both the 44-group library and the 238-group library. The DORT calculations used a P_3 cross-section expansion and an S_{16} angular quadrature. A total of 2000 generations with 5000 neutrons per generation were used in the KENO V.a calculations to obtain small statistical uncertainties. The DORT value of k_{eff} for the 238-group case agreed well with the KENO V.a result. The agreement is not as good for the 44-group cases with the KENO V.a result being 0.0016 higher. The 238-group DORT result is 0.0004 lower than the 44-group DORT result, while the 238-group KENO V.a result is 0.0016 lower than the 44-group KENO V.a result. This comparison does highlight a minor difference between DORT and KENO V.a results. However, the DORT results appear to be consistent. This indicates that the forward GIP cross-section file produced by SEN2 with filename fort.8 is correct. A P_5 calculation was also performed, and SEN2 works correctly for P_5.

The value of k_{eff} obtained from the adjoint DORT case is almost identical to the value obtained in the forward case. This agreement indicates that the adjoint GIP cross-section file produced by SEN2 with filename fort.18 is correct. In addition, the agreement is an indication that the angular quadrature and the spatial mesh used in the DORT calculation are adequate. P_5 cross sections also worked as expected.

Increasing and decreasing the ^{235}U atom density, as was done in Sect. 11, a value of 0.2458 was determined for the sensitivity of k_{eff} to changes in the ^{235}U atom density. This direct-calculation result compares very well with the perturbation theory result of 0.2454 calculated by LAKE. This agreement is an indication that VIP2D is programmed correctly. In addition, the 2-D sensitivity calculations were repeated using a P_5 cross-section expansion. This procedure tests both the adequacy of using P_3 cross sections and the adequacy of using P_3 flux

moments to calculate the perturbation term discussed in the previous section. The ^{235}U number density sensitivity is the same for both the P_3 and the P_5 calculation. This agreement indicates that P_3 DORT calculations are adequate for this sensitivity.

Table A.5.1 Calculated values of k_{eff} for Sheba 2

Case	Code	Groups	k_{eff}
Base case - forward	DORT	44	1.00275
Base case - adjoint	DORT	44	1.00276
U-235 density increased 4%	DORT	44	1.01232
U-235 density decreased 4%	DORT	44	0.992604
Base case - forward	KENO V.a	44	1.0044 +/- 0.0003
Base case - forward	DORT	238	1.00235
Base case - forward	KENO V.a	238	1.0028 +/- 0.0003

REFERENCES

A.1 R. L. Childs, D. E. Bartine, and W. W. Engle, "Perturbation Theory and Sensitivity Analysis for Two-Dimensional Shielding Calculations," *Trans. Am. Nucl. Soc.* **21,** 543–544 (1975).

INTERNAL DISTRIBUTION

1. S. M. Bowman
2–6. B. L. Broadhead (5)
7–10. W. C. Carter (4)
11–15. R. L. Childs (5)
16. M. E. Dunn
17. M. D. DeHart
18. K. R. Elam
19. M. B. Emmett
20. N. M. Greene
21. G. R. Handley
22. O. W. Hermann
23. D. F. Hollenbach
24. C. M. Hopper
25. W. C. Jordan
26. M. A. Kuliasha
27. L. C. Leal
28. J. F. Mincey
29–33. C. V. Parks (5)
34. L. M. Petrie
35. R. T. Primm
36. C. E. Pugh
37. B. T. Rearden
38. R. C. Robinson
39. R. W. Roussin
40. C. H. Shappert
41. R. G. Taylor
42. T. E. Valentine
43. R. M. Westfall
44. R. Q. Wright
45. Central Research Library, Document Reference Section
46. ORNL-Y-12 Technical Library
47–48. ORNL Laboratory Records (2) (for submission to OSTI)
49. ORNL Laboratory Records - RC
50. ORNL Patent Section

EXTERNAL DISTRIBUTION

51. F. M. Alcorn, BWX Technologies, Inc., Naval Nuclear Fuel, 212 Windsor Rd., Lynchburg, VA 24502
52. S. Almodovar, Fluor Daniel Hanford, P.O. Box 1000, Mail Stop A3-02, Richland, WA 99352-1000
53. S. Altschuler, U.S. Department of Energy, Richland Operations, 825 Jadwin, R3-79, Richland, WA 99352
54. R. E. Anderson, Los Alamos National Laboratory, P.O. Box 1663, NIS-6, MS J562, Los Alamos, NM 87545
55. W. L. Andrews, Defense Nuclear Facilities Safety Board, 625 Indiana Ave., Washington, DC 20004
56. C. Apperson, Westinghouse Savannah River Company, Savannah River Site, Bldg. 773-11A, Aiken, SC 29808-0001
57. M. G. Bailey, U.S. Nuclear Regulatory Commission, MS O6-G22, Washington, DC 20555
58. G. H. Bidinger, Nuclear Criticality Safety, 17016 Cashell Road, Rockville, MD 20853
59. R. N. Blomquist, Argonne National Laboratory, RA/208, 9700 S. Case Ave., Argonne, IL 60439-4842

60. C. Boman, BWX Technologies, Inc., Naval Nuclear Fuel, P.O. Box 785, Lynchburg, VA 24505
61. M. C. Brady Raap, Duke Engineering Services, 10503 W. Williams Road, Benton City, WA 99320
62. J. B. Briggs, INEEL, P.O. Box 1625, MS-3855, Idaho Falls, ID 83402
63. T. Burns, Defense Nuclear Facilities Safety Board, 625 Indiana Ave., Washington, DC 20004
64. R. D. Busch, University of New Mexico, Chemical and Nuclear Engineering Department, FEC 209, Albuquerque, NM 87131-1341
65. D. E. Cabrilla, U.S. DOE EM-66, Nuclear Material Stabilization, 19901 Germantown Road, Germantown, MD 20874-1290
66. D. E. Carlson, U.S. Nuclear Regulatory Commission, MS O6-F18, Washington, DC 20555
67. K. J. Carroll, Lockheed Martin Energy Systems, Y-12 Plant, P.O. Box 2009, Oak Ridge, TN 37831-8238
68. P. Cousinou, Institute of Protection and Nuclear Safety, B. P. 6 - 92265 Fontenay-Aux-Roses, Cedex, France
69. D. R. Damon, U.S. Nuclear Regulatory Commission, MS T8-H7, Washington, DC 20555
70. J. R. Davis, U.S. Nuclear Regulatory Commission, MS T8-A33, Washington, DC 20555
71. J. W. Davis, Framatome Cogema Fuels, CRWMS M&O, 1261 Town Center Dr., Las Vegas, NV 89134
72. R. L. Dintaman, U.S. Department of Energy, DP-13, 19901 Germantown Rd., Germantown, MD 20874-1290
73. H. L. Dodds, University of Tennessee, Nuclear Engineering Dept., 214 Pasqua Engineering Bldg., Knoxville, TN 37922
74. T. W. Doering, Framatome Cogema Fuels, 1261 Town Center Drive, Las Vegas, NV 89124
75. F. Eltawila, U.S. Nuclear Regulatory Commission, MS T10-E46, Washington, DC 20555
76. J. D. Evans, U.S. Department of Energy, S-3.1/VISTA, 1000 Independence Ave., S.W., Washington, DC 22085
77. H. D. Felsher, U.S. Nuclear Regulatory Commission, MS T8-H7, Washington, DC 20555
78. P. Felsher, Rocky Flats Environment Technology Site, Bldg. T886B, P.O. Box 464, Golden, CO 80402-0464
79. J. R. Felty, Science Applications Int'l Corp., 2418 N. Dickerson St., Arlington, VA 22207
80. I. E. Fergus, U.S. Department of Energy, EH-22, 20300 Century Blvd., Germantown, MD 20874
81. P. Finck, Argonne National Laboratory, 9700 South Cass Avenue, RA/208, Argonne, IL 60439-4842
82. E. K. Fujita, Argonne National Laboratory, 9700 South Cass Avenue, RA/208, Argonne, IL 60439-4842
83. A. S. Garcia, U.S. Department of Energy, Idaho Operations Office, 850 Energy Dr., MS 1154, Idaho Falls, ID 83401-1563
84. E. Greenspan, University of California, 4101 Etchevenny Hall, Berkeley, CA 94720
85. J. Gulliford, AEA Technology Engineering Services, Inc., 241 Curry Hollow Road, Pittsburgh, PA 15236-4696
86. D. K. Hays, Los Alamos National Laboratory, P. O. Box 1663, Los Alamos, NM 87545
87. D. Heinrichs, Lawrence Livermore National Laboratory, P.O. Box 808, MS L-128, Livermore, CA 94551

88. A. B. Hoffman, Lockheed Martin Idaho Tech. Co., P.O. Box 1625, MS 3458, Idaho Falls, ID 83415-3458
89. S. T. Huang, Lawrence Livermore National Laboratory, MS L-128, P.O. Box 808, Livermore, CA 94551
90. J. C. Ingram, Bechtel Jacobs Company LLC, P. O. Box 4699, Bldg. K-1320, MS-7592, Oak Ridge, TN 37831-7592
100. E. F. Kendall, U.S. Department of Energy, Oak Ridge Operations Office, YSO, P.O. Box 2001, Oak Ridge, TN 37831
101. K. D. Kimball, NISYS Corporation, 6055 Atlantic Blvd., Suite G-2, Norcross, GA 30071
102. R. P. Koopman, Lawrence Livermore National Lab., P.O. Box 808, L-467, Livermore, CA 94551
103. M. A. Lee, U.S. Department of Energy, Livermore Operations, 7000 East St., P.O. Box 808, L-293, Livermore, CA 94551-0808
104. R. Libby, Pacific Northwest National Laboratory, P.O. Box 999, M/S K7-74, Richland, WA 99352
105. J. J. Lichtenwalter, Bechtel Jacobs Company LLC, P.O. Box 4699, Bldg. K-1320, MS-7592, Oak Ridge, TN 37831-7592
106. R. C. Little, Los Alamos National Laboratory, MS F663, P.O. Box 1663, Los Alamos, NM 87545
107. C. D. Manning, Siemens Power Corporation, 2101 Horn Rapids Road, P.O. Box 130, Richland, WA 99352-0130
108. R. McBroom, U.S. Department of Energy, Oak Ridge Operations Office, YSO, P.O. Box 2001, Oak Ridge, TN 37831
109. J. McKamy, U.S. Department of Energy, EH-34, 19901 Germantown Road, Germantown, MD 20874-1290
110. R. D. McKnight, Argonne National Laboratory, 9700 S. Cass Ave., Argonne, IL 60439-4842
111. T. P. McLaughlin, Los Alamos National Laboratory, P. O. Box 1663, Los Alamos, NM 87545
112. D. E.I. Mennerdal, E M Systems, Starvãgen 12, Täby, SWEDEN S-18357
113. R. D. Montgomery, Nuclear Fuel Services, Inc., 1205 Banner Hill Rd., Erwin, TN 37650
114. D. C. Morey, U.S. Nuclear Regulatory Commission, MS T8-A33, Washington, DC 20555
115. J. A. Morman, Argonne National Laboratory, 9700 S. Cass Ave., Bldg. 208, C237B, Argonne, IL 60439-4842
116. R. D. Mosteller, Los Alamos National Laboratory, MS J562, Los Alamos, NM 87545
117. K. A. Niemer, Duke Engineering & Services, 400 S. Tryon St., WC26B, P.O. Box 1004, Charlotte, NC 28201-1004
118. C. W. Nilsen, U.S. Nuclear Regulatory Commission, MS T9-F31, Washington, DC 20555
119. H. Okuno, Japan Atomic Energy Research Institute, 2-4 Shirakara-shirane, Tokai-mura, Ibaraki-ken, JAPAN 319-1195
120. S. A. Parra, Lawrence Livermore National Laboratory, P.O. Box 808, MS L-128, Livermore, CA 94551
121. L. E. Paulson, Manager, Nuclear Safety, GE Nuclear Energy, P.O. Box 780, Castle Hayne Road, Wilmington, NC 28405
122. S. Payne, U.S. DOE/AL/SASD, P.O. Box 5400, Albuquerque, NM 87185-5400
123. V. A. Perin, U.S. Nuclear Regulatory Commission, NMSS/DWM, MS T7-F3, Washington, DC 20555

124. J. Person, Lawrence Livermore National Laboratory, P.O. Box 808, MS L-128, Livermore, CA 94551
125. R. E. Pevey, University of Tennessee, Nuclear Engineering Dept., 214 Pasqua Engineering Bldg., Knoxville, TN 37922
126. J. Philbin, Sandia National Laboratory, P.O. Box 5800, Albuquerque, NM 87185-1143
127. A. W. Prichard, Pacific Northwest National Laboratory, P.O. Box 999, MSIN: K8-34, Richland, WA 99352
128. M. Rahimi, U.S. Nuclear Regulatory Commission, M/S T7F3, Washington, DC 20555
129. T. A. Reilly, Westinghouse Safety Management Solutions, 1993 South Centennial Dr., Aiken, SC 29803
130. J. D. Roarty, Defense Nuclear Facilities Safety Board, 625 Indiana Ave., N.W., Suite 700, Washington, DC 2004
131. C. Rogers, Duke Engineering Services, 10503 W. Williams Road, Benton City, WA 99320
132. C. T. Rombough, CTR Technical Services, Inc., 950 Sugarloaf Rd., Manitou Springs, CO 80829
133. B. Rothleder, U.S. Department of Energy, EH-31, 19901 Germantown Rd., Germantown, MD 20874-1290
134. M. K. Sheaffer, Lawrence Livermore National Laboratory, P.O. Box 808, L-634, Livermore, CA 94550
135. G. L. Stimmell, Manager, General Electric Co., Vallecitos Nuclear Center, P.O. Box 460, Vallecitos Road, Pleasanton, CA 94566
136. J. T. Taylor, Principle Engineer - CSE, GE Nuclear Energy, P.O. Box 780, Castle Hayne Road, Wilmington, NC 28402
137. T. Taylor, Lockheed Martin Idaho Tech. Co., P.O. Box 1625, MS 3458, Idaho Falls, ID 83415-3458
138. D. A. Thomas, Framatome Cogema Fuels, 1261 Town Center Drive, Las Vegas, NV 89124
139. C. Tripp, U.S. Nuclear Regulatory Commission, MS T8-A33, Washington, DC 20555
140. H. Toffer, Fluor Daniel Northwest, Inc., P.O. Box 1050, MSIN B4-44, 1100 Jadwin Ave., Richland, WA 99352-1050
141. E. F. Trumble, Westinghouse Safety Management Solutions, P.O. Box 5388, 1993 South Centennial Dr., Aiken, SC 29803
142. J. J. Wagschal, Racah Institute of Physics, The Hebrew University of Jerusalem, 91904, Jerusalem, ISRAEL
143. M. Wangler, Office of Site Operations, EM-70/CLV-1059, U.S. Department of Energy, 19901 Germantown Road, Germantown, MD 20874-1290
144. L. Wetzel, BWX Technologies, Inc., Naval Nuclear Fuel, P.O. Box 785, Lynchburg, VA 24505
145. S. A. Whaley, U.S. Nuclear Regulatory Commission, MS O6-G22, Washington, DC 20555
146. B. H. White IV, U.S. Nuclear Regulatory Commission, MS O6-F18, Washington, DC 20555
147. D. W. Williams, Westinghouse Electric Corporation, 5801 Bluff Rd MS#15, Columbia, SC 29209
148. Mark Williams, Louisiana State University, Baton Rouge, LA 70803-5820
149. R. E. Wilson, Safe Sites of Colorado, P.O. Box 464, Golden, CO 80402-0464
150. C. J. Withee, U.S. Nuclear Regulatory Commission, MS O6-G22, Washington, DC 20555

NRC FORM 335 (2-89)
NRCM 1102
3201, 3202

U.S. NUCLEAR REGULATORY COMMISSION

BIBLIOGRAPHIC DATA SHEET

(See instructions on the reverse)

1. REPORT NUMBER (Assigned by NRC, Add Vol., Supp., Rev., and Addendum Numbers, if any.)

NUREG/CR-5719
ORNL/TM-13738

2. TITLE AND SUBTITLE

SEN1: A One-Dimensional Cross-Section Sensitivity and Uncertainty Module for Criticality Safety Analysis

3. DATE REPORT PUBLISHED

MONTH	YEAR
July	1999

4. FIN OR GRANT NUMBER

W6479

5. AUTHOR(S)

R. L. Childs

6. TYPE OF REPORT

Technical

7. PERIOD COVERED *(Inclusive Dates)*

September 1995 - March 1999

8. PERFORMING ORGANIZATION — NAME AND ADDRESS *(If NRC, provide Division, Office or Region, U.S. Nuclear Regulatory Commission, and mailing address; if contractor, provide name and mailing address.)*

Oak Ridge National Laboratory
Post Office Box 2008
Oak Ridge, TN 37831-6370

9. SPONSORING ORGANIZATION — NAME AND ADDRESS *(If NRC, type "Same as above"; if contractor, provide NRC Division, Office or Region, U.S. Regulatory Commission, and mailing address.)*

Division of Systems Analysis and Regulatory Effectiveness
Office of Nuclear Regulatory Research
U.S. Nuclear Regulatory Commission
Washington, DC 20555-0001

10. SUPPLEMENTARY NOTES

11. ABSTRACT *(200 words or less)*

This report documents sensitivity analysis computer codes that have been developed for use with one-dimensional (1-D) and two-dimensional (2-D) calculational models. These codes provide a useful tool to aid criticality safety analysts in understanding the applicability of selected critical experiments to the validation of real systems.

SEN1 is a prototypic SCALE control module that facilitates the application of sensitivity theory to criticality safety analysis. The XSDRNPM module uses the method of discrete ordinates to calculate k_{eff} for applications that are appropriate for 1-D modeling. Perturbation theory is used to determine the sensitivity of the calculated value of k_{eff} to the nuclear data used in the calculation as a function of nuclide, reaction type, and energy. The uncertainty in the calculated value of k_{eff}, resulting from uncertainties in the basic nuclear data used in the calculation, is estimated using energy-dependent relative covariance matrices processed from ENDF/B-V. Systems containing arrays of fuel pins may be analyzed using cell-weighted cross sections. The methods used in this work are based on the FORSS system developed at ORNL in the 1970s. The present work uses the XSDRNPM module and the problem-dependent cross-section processing capabilities of the SCALE system and is much more automated than the earlier FORSS system. Two-dimensional sensitivity analysis using the DORT code has also been developed and is described in the appendix.

12. KEY WORDS/DESCRIPTORS *(List words or phrases that will assist researchers in locating the report.)*

sensitivity, uncertainty, SCALE, criticality safety, FORSS

13. AVAILABILITY STATEMENT

Unlimited

14. SECURITY CLASSIFICATION

(This Page) Unclassified

(This Report) Unclassified

15. NUMBER OF PAGES

16. PRICE