LA-UR--82-2529

DE92 022021

TITLE: TWO-DIMENSIONAL CROSS-SECTION AND SED UNCERTAINTY ANALYSIS
FOR THE FUSION ENGINEERING DEVICE (FED)

AUTHOR(S): M. J. Embrechts, W. T. Urban, and Donald J. Dudziak

SUBMITTED TO: NUCLEAR DATA FOR SCIENCE AND TECHNOLOGY INTERNATIONAL CONFERENCE
6-10 September 1982

MASTER

By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes.

The Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy.

Los Alamos Los Alamos National Laboratory
Los Alamos, New Mexico 87545

TWO-DIMENSIONAL CROSS-SECTION AND SED UNCERTAINTY ANALYSIS FOR THE FUSION ENGINEERING DEVICE (FED)

M. J. Embrechts and W. T. Urban

Theoretical Division
University of California
Los Alamos National Laboratory
P. O. Box 1663
Los Alamos, New Mexico 87545 USA

Donald J. Dudziak

EIR - Switzerland
Eidg. Institut für Reaktorforschung
CH-5303 Würenlingen
Switzerland

The theory of two-dimensional cross-section and secondary-energy-distribution (SED) sensitivity was implemented by developing a two-dimensional sensitivity and uncertainty analysis code, SENSIT-2D. Analyses of the Fusion Engineering Design (FED) conceptual inboard shield indicate that, although the calculated uncertainties in the 2-D model are of the same order of magnitude as those resulting from the 1-D model, there might be severe differences. The more complex the geometry, the more compulsory a 2-D analysis becomes. Specific results show that the uncertainty for the integral heating of the toroidal field (TF) coil for the FED is 114.6%. The main contributors to the cross-section uncertainty are chromium and iron. Contributions to the total uncertainty were smaller for nickel, copper, hydrogen and carbon. All analyses were performed with the Los Alamos 42-group cross-section library generated from ENDF/B-V data, and the COVFILS covariance matrix library. The large uncertainties due to chromium result mainly from large covariances for the chromium total and elastic scattering cross sections.

Introduction

The calculation of nuclear design parameters is often limited in accuracy due to errors resulting from the calculational methods and the cross-section data utilized. Continuous developments in the calculational methods and computer codes accentuate the importance to improve the cross-section data. Cross-section sensitivity analysis^{1,2} has become a widely applied design tool which allows the user to pinpoint the most crucial partial cross sections in a specific energy range for a particular design. A cross-section sensitivity analysis leads to a broader interpretation of the results from a transport calculation and, in conjunction with an uncertainty analysis, provides a way to estimate errors for a particular response (e.g. nuclear heating, radiation damage, etc.). Consecutively, it can be determined where improvements in the nuclear data or in the design are needed to reduce that uncertainty. Secondary-energy-distribution sensitivity and uncertainty analysis^{3,4} becomes important for the study of threshold reactions, e.g., ${}^7\text{Li}(n,n'\alpha)\text{T}$, while design sensitivity analysis⁵ can lead to a significant reduction in the number of transport calculations required during the optimization process for a particular design. The complicated geometry of a fusion reactor makes the capability to undertake two-dimensional sensitivity analysis in a toroidally symmetric system highly desirable. Therefore, a two-dimensional sensitivity and uncertainty analysis code, SENSIT-2D,^{6,7} which can mock-up a toroidal geometry, was developed and applied to the FED.

Theory

The theory behind cross-section sensitivity and uncertainty analysis has been explained by several authors^{1,2} and involves the use of covariance matrices and sensitivity profiles. The variance of the response corresponding to two correlated cross-section uncertainties can be expressed by

$$\left(\frac{\Delta I}{I}\right)^2 = \sum_{i,j} P_{\Sigma_i} P_{\Sigma_j} \frac{\text{Cov}(\Sigma_i, \Sigma_j)}{\Sigma_i \Sigma_j}, \quad (1)$$

where I is the integral response, Σ_i and Σ_j are cross sections, P_{Σ_i} and P_{Σ_j} are sensitivity profiles of the integral response with respect to Σ_i and Σ_j , and $\text{Cov}(\Sigma_i, \Sigma_j)$ is the matrix of the covariance data. The first part in the above expression ($P_{\Sigma_i} P_{\Sigma_j}$) is highly problem dependent, while the second part requires cross-section uncertainty information and is problem independent.

The sensitivity profiles are defined as the fractional change of the integral response per fractional change of cross-section, normalized per lethargy width. Sensitivity profiles can be calculated based on forward and adjoint angular fluxes. Cross-section covariance data describe the uncertainties in multigroup cross-section data and the correlation between those uncertainties. A non-zero non-diagonal covariance matrix element indicates that there was a common reason why an uncertainty in two different cross sections was introduced. Multigroup covariance data are ordered in covariance matrices. Such a covariance matrix contains GMAX rows and GMAX columns, where GMAX is the number of energy groups. A covariance matrix can contain covariance data of a particular partial cross section with itself over an energy range, with a different partial cross section for the same element, or with a partial cross section for a different element. A 30-group covariance library, COVFILS, based on ENDF/B-V which contains most of the elements commonly used in fusion reactor shielding has been constructed by Muir and LaBauve.⁸ The covariance data in this library were processed by using the NJOY code.⁹

By introducing the "hot-cold" and "forward-backward" concepts, Gerstl^{3,4} developed a framework which leads to expressions similar to Eq. (1) for calculating uncertainties due to uncertainties in secondary energy (SED) and secondary angular (SAD) distributions. For a SED uncertainty calculation a median energy group which distributes the secondary energy neutrons in a "hot" and a "cold" part is defined as the group into which the median energy of the secondary energy distribution falls. An integral SED profile is then defined which can be hot or cold depending whether the response is more sensitive to the "hot" secondary neutrons than to the "cold" ones. The equivalent of the covariance data in Eq. (1) are the fractional un-

the spectral shape for the secondary energy distribution. The fractional uncertainties for some materials have been evaluated.¹⁰ All secondary particle production processes for a particular element are presently treated as one single process. The simplicity of the "hot-cold" concept and the fact that all secondary particle production processes for a particular element are treated as one single process might be causes for an underestimation of the SED uncertainties.

In principle similar algorithms for calculating uncertainties due to uncertainties in the secondary angular distribution can be constructed using the "forward-backward" formalism. However, the necessary data haven't been evaluated yet.

SENSIT-2D

SENSIT-2D, which is an extension of the one-dimensional sensitivity code SENSIT,¹¹ has the capability for cross-section sensitivity and uncertainty analysis, SED sensitivity and uncertainty analysis and design sensitivity analysis. The algorithms utilized are based on first-order generalized perturbation theory. The code allows (x,y) or (r,z) geometry options and accepts group-dependent quadrature sets. It is intended for use with the two-dimensional, multigroup, discrete-ordinates transport code TRIDENT-CTR.¹² The triangular mesh used by TRIDENT-CTR allows unique modeling capabilities that are applicable to fusion reactor configurations, and thus SENSIT-2D can also analyze these configurations. The forward and adjoint angular fluxes generated by TRIDENT-CTR are required input to SENSIT-2D. Because the number of angular fluxes can be voluminous, a sophisticated data management scheme was necessary for the code to keep the execution time and memory requirements within reasonable limits.

The computational outline for a two-dimensional sensitivity analysis with SENSIT-2D is shown in Fig. 1. There are three major parts: a cross section preparation block which prepares cross sections and covariance data, a transport block which includes a forward and an adjoint transport calculation and a postprocessing of the angular fluxes, and a sensitivity block, which performs the sensitivity and uncertainty calculations.

Cross-Section and SED Uncertainty Analysis for the FED

Two-dimensional cross-section and SED sensitivity and uncertainty analyses of the integral heating in the

inboard toroidal field coil of the FED conceptual design were performed. The TRIDENT-CTR forward and adjoint calculations used 30 neutrons and 12 gamma-ray groups, a P_3 scattering approximation and a group dependent quadrature set. The cross-section library used was based on ENDF/B-V data. The calculational model is shown in Fig. 2 and was based on the latest FED data available at the start of this effort.

The SENSIT-2D calculations were performed using the COVFILS⁶ covariance matrix library which is based on ENDF/B-V data. Covariance data for copper are based on those for iron. The SED data used in this analysis were obtained from Reference 10. Because the elastic scattering cross-section data for hydrogen are well known and due to the lack of SED data for hydrogen, hydrogen was not considered for calculating uncertainties resulting from uncertainties in the SEDs. It was assumed that the uncertainties for a particular element in the various SS 316 zones are fully correlated, while all other uncertainties are assumed to be uncorrelated.

Results from this study are shown in Table 1. The overall uncertainty for the heating of the TF coil (at one standard deviation) is 115% and is in reasonable agreement with the 132% overall uncertainty obtained from a one-dimensional analysis reported elsewhere.¹³ It can be concluded that the cross-section uncertainties (predicted to be 113%) tend to be more important than the SED uncertainties (20%). The major contributors to the cross-section uncertainty are chromium with relative standard deviations of 96.7% and 47.3%, respectively. The corresponding values for SED uncertainties are 4.9% and 18.4%. Contributions to the total uncertainty were smaller for nickel, copper, hydrogen and carbon. A more detailed look at the computer listings generated by this analysis reveals that the largest uncertainties are produced by uncertainties in the total and the elastic scattering cross sections for chromium, and that the heating is less sensitive to chromium than to iron. This indicates that the calculated uncertainty is largely due to the fact that chromium has very large covariances. A re-evaluation of the covariance data for chromium is therefore recommended. If new covariance data would not reduce the predicted uncertainty, new experiments for measuring the chromium cross sections are suggested.

The SED uncertainties, although less relevant to the overall predicted uncertainty, tend to become more important in the outboard shield. A possible explanation for this behavior is related with the fact that the heating in the TF-coil will be very sensitive to

Fig. 1. Computational outline for a two-dimensional sensitivity

Fig. 2. FED calculational model.

TABLE I

PREDICTED UNCERTAINTIES (STANDARD DEVIATION) DUE TO ESTIMATED SED AND CROSS-SECTION UNCERTAINTIES FOR THE HEATING IN THE TF COIL FROM A TWO-DIMENSIONAL ANALYSIS

Cross Section		SED Uncertainties in %		XS Uncertainties in %	
Material	Zone	$\left[\frac{\Delta R}{R}\right]_{\text{Mat,region}}$	$\left[\frac{\Delta P}{R}\right]_{\text{Mat}}$	$\left[\frac{\Delta R}{R}\right]_{\text{Mat,region}}$	$\left[\frac{\Delta P}{R}\right]_{\text{Mat}}$
Cr	SS316	3.8	4.9	60.0	96.7
	TF COIL	0.2		34.5	
	SS304	0.1		4.5	
	SS312	0.0		1.1	
	ISDLC	0.2		2.2	
	ISDLB	0.8		33.3	
	ISDLA	3.0		58.5	
Fe	SS316	14.8	18.4	18.9	47.3
	TF COIL	0.1		10.4	
	SS304	0.0		2.2	
	SS312	0.2		0.7	
	ISDLC	0.5		4.4	
	ISDLB	2.7		23.6	
	ISDLA	10.8		34.5	
Ni	SS316	1.5	4.3	18.6	31.4
	TF COIL	0.7		11.8	
	SS304	0.0		0.9	
	SS312	0.0		0.4	
	ISDLC	0.0		1.3	
	ISDLB	0.4		13.4	
	ISDLA	1.2		18.0	
H	TF COIL	-	-	1.7	7.2
	ISDLC	-		6.0	
	ISDLB	-		3.7	
	ISDLA	-		0.5	
O	TF COIL	0.1	0.3	-	-
	ISDLC	0.2		-	
	ISDLB	0.1		-	
	ISDLA	0.1		-	
C	TF COIL	0.0	0.3	0.1	3.2
	C-region	0.3		3.2	
Cu	TF COIL	2.9	2.9	10.1	10.1
Total ^a			19.7		112.9

Total uncertainty due to cross-section and SED uncertainties = 114.6%

^aQuadrature sum

SED uncertainties in this region. The SED uncertainties in the outboard shield were different from those obtained with the one-dimensional model. More relevant than the uncertainty of the integral heating of the TF coil would be the uncertainty of the hot-spot heating of the TF coil. However, the results of the hot-spot analysis are very similar to those reported in Table I, (less than 5% difference).

Conclusions

The two-dimensional sensitivity and uncertainty analysis code, SENSIT-2D, was applied to the FED. The overall uncertainty for the heating of the TF-coil was found to be 115% and mainly due to cross-section uncertainties, while the SED uncertainties were less important. The largest uncertainties were caused by uncertainties in the chromium and iron cross section. A re-evaluation of the covariance data for chromium might lead to smaller predicted uncertainties.

References

1. S. A. W. Gerstl, Donald J. Dudziak, and D. W. Muir, "Cross-Section Sensitivity and Uncertainty Analysis with Application to a Fusion Reactor," Nuclear Science and Engineering, 62, 137 (1977).
2. D. J. Dudziak, "Cross-Section Sensitivity and Uncertainty Analysis for Fusion Reactors (a Review)," Proceedings of the Advisory Group Meeting on Nuclear Data for Fusion Reactor Technology, IAEA, Vienna, Austria, 11-15 December 1978.
3. S. A. W. Gerstl, "Sensitivity Profiles for Secondary Energy and Angular Distributions," Proc. Fifth Int. Conf. Reactor Shielding, 18-23 April 1977, Knoxville, TN, Proceedings edited by R. W. Roussin et al., Science Press, Princeton (1978).
4. S. A. W. Gerstl, "Uncertainty Analysis for Secondary Energy Distributions," Proc. Seminar-Workshop on Theory and Application of Sensitivity and Uncertainty Analysis, 22-24 August 1978, Oak Ridge, TN, Proceedings edited by C. R. Weisbin et al., ORNL/RSIC-42 (February 1979).
5. E. L. Simmons, Donald J. Dudziak, and S. A. W. Gerstl, "Nuclear Design Sensitivity Analysis for a Fusion Reactor," Nuclear Technology, 34, 317 (1977).
6. M. J. Embrechts, "Two-Dimensional Cross-Section Sensitivity and Uncertainty Analysis for Fusion Reactor Blankets," Los Alamos National Laboratory report LA-9232-T (1982).
7. M. J. Embrechts, "SENSIT-2D: A Two-Dimensional Cross-Section Sensitivity and Uncertainty Analysis Code," Los Alamos National Laboratory report LA-9515-MS (1982).
8. D. W. Muir and R. J. LaBauve, "COVFILS A 30-Group Covariance Library Based on ENDF/B-V," Los Alamos National Laboratory report LA-8733-MS (1981).
9. R. E. MacFarlane, D. W. Muir and R. M. Boicourt, "The NJOY Nuclear Data Processing System, Volume I: User's Manual," Los Alamos National Laboratory report LA-9303-M (1982).
10. S. A. W. Gerstl, R. J. LaBauve and P. G. Young, "A Comprehensive Neutron Cross-Section and Secondary Energy Distribution Uncertainty Analysis for a Fusion Reactor," Los Alamos Scientific Laboratory report LA-8333-MS (1980).
11. S. A. W. Gerstl, "SENSIT: A Cross-Section and Design Sensitivity and Uncertainty Analysis Code," Los Alamos Scientific Laboratory report LA-8498-MS (1980).

12. J. J. Serp, "TRIDENT-UK User's Manual," Los Alamos National Laboratory report LA-7835-M (1979).
13. D. J. Dudziak, R. D. O'Dell, and R. E. Alcouffe, "Transport and Reactor Theory October 1 - December 31, 1981," Los Alamos National Laboratory report LA-9336-PR (1982).