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UNCERTAINTY ANALYSIS CODE SENSIT-2D WITH APPLICATIONS TO THE FED

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DEVELOPMENT OF THE TWO-DIMENSIONAL CROSS-SECTION SENSITIVITY
AND UNCERTAINTY ANALYSIS CODE SENSIT-2D WITH APPLICATIONS TO THE FED

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ABSTRACT

Sensitivity and uncertainty analyses implement the information obtained from a transport code by providing a reasonable estimate for the uncertainty of a particular design parameter and a better understanding of the nucleonics involved. The toroidal geometry of many fusion devices motivates a two-dimensional calculation capability. A two-dimensional cross-section and secondary energy distribution (SED) sensitivity and uncertainty analysis code, SENSIT-2D, has been developed that allows modeling of a toroidal geometry. Two-dimensional and one-dimensional sensitivity analyses for the heating and the copper d.p.a. of the TF coil for a conceptual FED blanket/shield design were performed. The uncertainties from the two-dimensional analysis are of the same order of magnitude as those obtained from the one-dimensional study. The largest uncertainties were caused by the cross-section covariances for chromium.

I. INTRODUCTION

The calculation of nuclear design parameters is often limited in accuracy due to errors resulting from calculational methods and the cross-section data utilized. Cross-section sensitivity analysis has become a widely applied design tool that allows the user to pinpoint the most crucial 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.). Consequently, it can be determined where improvements in the nuclear data and/or the design are needed to reduce that uncertainty. Those conclusions resulting from a sensitivity analysis are design dependent. That does not mean, however, that broader conclusions applicable to a generic class of similar designs cannot be drawn.

The complicated geometry of a fusion reactor makes the capability to undertake a two-dimensional sensitivity analysis in a toroidally symmetric system highly desirable. A two-dimensional code, SENSIT-2D,^{1,2} which can model a toroidal geometry, was developed and has been applied to a conceptual design for the FED blanket/shield. SENSIT-2D has the capability for cross-section sensitivity and uncertainty analyses, secondary-energy-distribution (SED) sensitivity and uncertainty analyses, and design sensitivity analyses. The algorithms utilized are based on first-order perturbation theory. The code allows x-y or r-z geometry options and accepts group dependent quadrature sets. SENSIT-2D is intended to be used in conjunction with the two-dimensional multigroup, discrete-ordinates transport code TRIDENT-CTR.³

The theory behind cross-section sensitivity and uncertainty analysis has been described elsewhere.⁴⁻⁸ In this paper we will give a brief review of the basic expressions, including those for secondary energy distribution sensitivity and uncertainty analysis. The structure of SENSIT-2D is highlighted and its applicability to a conceptual design for the FED blanket/shield is illustrated. Finally, the results from a two-dimensional cross-section sensitivity and uncertainty analysis are compared with those from a one-dimensional analysis for the heating and copper d.p.a. of the TF coil.

II. THEORY

The theoretical foundations for cross-section sensitivity and uncertainty analysis are well documented; therefore, only the key expressions will be repeated. Concentrating on a set of multigroup cross-section data, Σ_i , we are interested in an expression for the standard deviation, ΔR , of a design parameter R (e.g. nuclear heating, copper d.p.a., etc.). The concepts of covariance data and sensitivity profiles lead to a simple way to evaluate the error in R due to cross-section uncertainties, where ΔR can be

evaluated from

$$\left[\frac{\Delta R}{R}\right]_{xs}^2 = \sum_{g,i} P_{\Sigma_i^g} P_{\Sigma_j^g} \frac{\text{COV}(\Sigma_i^g, \Sigma_j^g)}{\Sigma_i^g \Sigma_j^g}. \quad (1)$$

In this expression Σ_i^g represents the interaction cross-section for type i in energy group g , $\text{COV}(\Sigma_i^g, \Sigma_j^g)$ is the covariance matrix for the multigroup cross sections Σ_i^g and Σ_j^g and $P_{\Sigma_i^g}$ is the relative sensitivity profile of the design parameter R for cross section Σ_i^g . $P_{\Sigma_i^g}$ is defined by

$$P_{\Sigma_i^g} = \frac{\partial R/R}{\partial \Sigma_i^g / \Sigma_i^g}. \quad (2)$$

Note that in Eq. (1) the first part of the summation, $P_{\Sigma_i^g} P_{\Sigma_j^g}$ is problem dependent, while the second part requires cross-section uncertainty information and is problem independent. The procedure to derive explicit expressions for the relative sensitivity profiles is straightforward. In the final stage it is necessary to evaluate $P_{\Sigma_i^g}$ and $P_{\Sigma_j^g}$ numerically, and different expressions for one-dimensional and two-dimensional treatments will be obtained.

By introducing the "hot-cold" concept Gerstl^{9,10} indicated that the uncertainty in the integral response due to uncertainties in the secondary energy distribution can be expressed in a similar way leading to

$$\left[\frac{\Delta R}{R}\right]_{xs}^2 = \sum_{g,i} S_{SED}^{g,i} S_{SED}^{g,j} \text{COV}(f_i^g, f_j^g), \quad (3)$$

where $S_{SED}^{g,i}$ is the integral SED sensitivity for cross section type i in energy group g , and f_i^g is the spectral shape uncertainty parameter for a specific nuclear reaction, e.g. $(n,2n)$, at a

specific incident neutron energy g . Assuming no correlation between f_i^g and f_j^g it can be shown that Eq. (3) simplifies to

$$\left[\frac{\Delta R}{R}\right]_{xs}^2 = \left[\sum_g S_{SED}^{g,i} \text{Var}(f_i^g) \right]. \quad (4)$$

$\text{Var}(f_i^g)$ is called the fractional uncertainty for the secondary energy distribution. A program that evaluates $\text{Var}(f_i^g)$ for various elements is available.¹¹ The overall response uncertainty due to cross-section uncertainties and secondary-energy-distribution uncertainties will be of the form

$$\left[\frac{\Delta R}{R}\right]^2 = \sqrt{\left[\frac{\Delta R}{R}\right]_{xs}^2 + \left[\frac{\Delta R}{R}\right]_{SED}^2}. \quad (5)$$

In principle similar algorithms for calculating uncertainties due to uncertainties in the secondary angular distribution can be constructed.

III. SENSIT-2D

The theory outlined in Sec. II has been incorporated in a two-dimensional cross-section and design sensitivity and uncertainty analysis code, SENSIT-2D. SENSIT-2D has the capability to perform a standard cross-section sensitivity and uncertainty analysis, a secondary energy distribution sensitivity and uncertainty analysis, a design sensitivity analysis and an integral response sensitivity and uncertainty analysis. As a special feature in the code, the loss term of the sensitivity profile can be evaluated based on angular fluxes and/or flux moments.¹² A description of the features of SENSIT-2D is summarized in Table I.

TABLE I: Summary of the Features of SENSIT-2D.

Code Information

- * written for a CDC-7600
- * typical storage 20K(SCH), 80K(LCM)
- * to be used with the TRIDENT-CTR transport code

Capabilities

- * computes the sensitivity and uncertainty of a calculated integral response due to input cross sections and their uncertainties
- * design sensitivity analysis
- * cross-section sensitivity and uncertainty analysis
- * secondary-energy distribution (SED) sensitivity and uncertainty analysis

TRIDENT-CTR Features Carried Over into SENSIT-2D:

- * x-y or r-z geometry
- * group-dependent S_n order
- * triangular spatial mesh

Limitations

- * can only interact with TRIDENT-CTR transport code
- * based on first-order perturbation theory
- * upscattering not allowed

SENSIT-2D is developed with the purpose of interacting with the TRIDENT-CTR³ code, a two-dimensional discrete-ordinates transport code with triangular meshes and an r-z geometry capability, tailored to the needs of the fusion community. Angular fluxes generated by other 2-D codes, such as DOT, TWODANT, TRIDENT, etc., cannot at present be accepted by SENSIT-2D due to the different format. The unique features of TRIDENT-CTR (group dependent quadrature sets, r-z geometry description, triangular meshes) are reflected in SENSIT-2D. Coupled neutron/gamma-ray studies can be performed. In contrast with TRIDENT-CTR however, SENSIT-2D is restricted to the use of equal weight (EQ_n) quadrature sets,¹³ symmetrical with respect to the four quadrants. Upscattering is not allowed.

Figure 1 presents a flow chart illustrating the outline for a two-dimensional sensitivity and uncertainty analysis with SENSIT-2D. From this figure, it becomes immediately

Fig. 1. Computational outline to do a two-dimensional sensitivity analysis with SENSIT-2D.

apparent that a sensitivity analysis requires elaborate data management. The data flow can be divided into three major parts: a cross-section preparation module, in which the cross-sections required by TRIDENT-CTR and SENSIT-2D are prepared, a TRIDENT-CTR/TRDSEN block where the angular fluxes in a form compatible with SENSIT-2D are generated, and a SENSIT-2D module, which performs the calculations and manipulations necessary for a sensitivity and uncertainty analysis.

There are many possible ways to generate the multigroup cross-section tables required by SENSIT-2D and TRIDENT-CTR. The flow chart of Fig. 1 illustrates just one of these possibilities. All the codes mentioned here are accessible via the MFECC. Basically, three codes are required: NJOY,¹⁴ TRANSX,¹⁵ and MIXIT.¹⁵ Starting from the ENDF/B-V data file, the NJOY code system generates a multigroup cross-section library (MATXS5) and a vector cross-section and covariance library (TAPE10). A covariance library can be constructed by using the ERRORR module in the NJOY code system. From the multigroup cross-section library (MATXS5), the desired isotopes can be extracted by the TRANSX code. The MIXIT code can make up new materials by mixing isotopes from the XSLIB5 library. The cross sections used in SENSIT-2D have to be written

on a file called TAPE4. The cross sections used in TRIDENT-CTR and TRDSEN will be on file GEODXS. SENSIT-2D and TRIDENT-CTR include the option to feed in cross sections directly from cards.

SENSIT-2D requires regular angular fluxes at the triangle centerpoints, multiplied by the corresponding volumes, and adjoint angular fluxes at the triangle centerpoints. TRIDENT-CTR does not write out angular fluxes. Therefore the TRDSEN postprocessor was developed, which makes use of the flux moment dump files generated by TRIDENT-CTR. These dump files will be the starting flux guesses for TRDSEN. TRDSEN will perform one more iteration and write out the angular fluxes. Except for a different starting guess option, TRDSEN requires the same input as TRIDENT-CTR.

IV. APPLICATION OF SENSIT-2D TO THE FED BLANKET/SHIELD

Two-dimensional and one-dimensional cross-section and SED sensitivity and uncertainty analyses of the heating and the copper d.p.a. in the inboard toroidal field coil of a FED conceptual design were performed. An r-z geometry representation for the FED is reproduced in Fig. 2. The TRIDENT-CTR calculation used 30 neutron and 12 gamma-ray groups, a P₃

Fig. 2. FED calculational model.

scattering calculation and an energy-dependent quadrature set. All analyses were performed with the Los Alamos 42-group MATXS cross-section library (ENDF/B-V), and the COVFILS covariance matrix library.¹⁶ The results from a two-dimensional sensitivity and uncer-

tainty analysis for the overall heating in the TF-coil for the FED conceptual design are illustrated in Table IIa. The corresponding data obtained from a one-dimensional sensitivity and uncertainty analysis, using ONEDANT and SENSIT, are summarized in Table IIb. The

TABLE II a
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	$\left[\frac{\Delta R}{R}\right]$	$\left[\frac{\Delta R}{R}\right]^a$	$\left[\frac{\Delta R}{R}\right]$	$\left[\frac{\Delta R}{R}\right]^a$
		Mat, region	Mat	Mat, region	Mat
Cr	SS316	3.8		60.0	
	TFCOIL	0.2		34.5	
	SS304	0.1		4.5	
	SS312	0.0	4.9	1.1	96.7
	ISDLC	0.2		2.2	
	ISDLB	0.8		33.3	
	ISDLA	3.0		58.5	
Fe	SS316	14.0		18.9	
	TFCOIL	0.1		10.4	
	SS304	0.0		2.2	
	SS312	0.2	18.4	0.7	47.3
	ISDLC	0.5		4.4	
	ISDLB	2.7		23.6	
	ISDLA	10.8		34.5	
Ni	SS316	1.5		18.6	
	TFCOIL	0.7		11.8	
	SS304	0.0		0.9	
	SS312	0.0	4.3	0.4	31.4
	ISDLC	0.0		1.3	
	ISDLB	0.4		13.4	
	ISDLA	1.2		18.0	
H	TFCOIL	-	-	1.7	
	ISDLC	-	-	6.0	7.2
	ISDLB	-	-	3.7	
	ISDLA	-	-	0.5	
O	TFCOIL	0.1		-	
	ISDLC	0.2	0.3	-	-
	ISDLB	0.1		-	
	ISDLA	0.1		-	
C	TFCOIL	0.0		0.1	
	C-region	0.3	0.3	3.2	3.2
Cu	TFCOIL	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% ^a					

^aQuadratic Sums.

TABLE II b

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

Cross-Section		SED Uncertainties in %		XS Uncertainties in %	
Material, Zone		$\left[\frac{\Delta R}{R}\right]$ Mat, region	$\left[\frac{\Delta R}{R}\right]$ Mat	$\left[\frac{\Delta R}{R}\right]$ Mat, region	$\left[\frac{\Delta R}{R}\right]$ Mat
Cr	SS316	2.1	3.8	85.9	115.9
	TFCOIL	0.2		52.3	
	SS304	0.1		4.4	
	SS312	0.0		1.2	
	ISDLC	0.2		1.7	
	ISDLB	0.8		27.2	
	ISDLA	3.0		50.6	
Fe	SS316	8.1	13.6	33.6	48.9
	TFCOIL	1.3		7.1	
	SS304	0.5		1.7	
	SS312	0.2		0.6	
	ISDLC	0.4		3.6	
	ISDLB	2.5		18.9	
	ISDLA	10.5		29.0	
Ni	SS316	1.7	2.2	28.1	37.2
	TFCOIL	0.6		14.9	
	SS304	0.1		1.4	
	SS312	0.0		0.4	
	ISDLC	0.1		1.1	
	ISDLB	0.3		10.8	
	ISDLA	1.3		16.0	
H	TFCOIL	-		1.9	6.1
	ISDLC	-		4.9	
	ISDLB	-		3.0	
	ISDLA	-		0.4	
O	TFCOIL	1.5	1.5	-	
	ISDLC	0.2		-	
	ISDLB	0.2		-	
	ISDLA	0.1		-	
C	TFCOIL	0.0	0.2	0.2	2.9
	C-region	0.2		2.9	
Cu	TFCOIL	4.7	4.7	10.5	10.5
Total ^a			15.1		131.8
Total uncertainty due to cross-section uncertainties and SEDs = 131.8% ^a					

^a Quadratic sums.

one-dimensional calculation was done with an eighth-order Gaussian quadrature set. The source was normalized such that the heating in the TF coil matches the heating from the TRIDENT-CTR calculation. The results from the

one-dimensional study are generally in agreement with those from the two-dimensional analysis, the total uncertainty in the two-dimensional analysis amounts to 115%, versus 132% for the one-dimensional calculation.

Specific two-dimensional results show that the major contribution to the cross-section uncertainty are chromium and iron, with relative standard deviations of 96.7% and 47.3%, respectively, in the TF-coil integral heating. Corresponding values for the SED uncertainties are 4.9% and 18.4%. Contributions to the total uncertainty were smaller for nickel, copper, hydrogen, and carbon. Results for a similar study of the hot-spot heating in the TF coil were within 2% of those for the integral heating.

A comparison between the 1-D and 2-D cross-section and SED uncertainties for the copper d.p.a. in the hot spot of the TF coil is made in Table III, leading to a total uncertainty of 73% and 54%, respectively.

There is good qualitative agreement between the results of the one-dimensional and two-dimensional analysis; the largest discrepancy is due to the difference of the contribution of chromium to the uncertainty. In the two-dimensional analysis iron is the major contributor to the overall uncertainty, while chromium causes the largest uncertainties in the one-dimensional analysis. A closer look at the computer data indicated that the sensitivity profiles for iron were much smaller than the corresponding profiles for chromium. The large uncertainties due to chromium result mainly from large covariances for the chromium total and scattering cross sections, and indicate a need for the re-evaluation of the covariances for chromium.

TABLE III
RESPONSE UNCERTAINTIES DUE TO CROSS-SECTION AND
SED UNCERTAINTIES FOR THE COPPER d.p.a. IN THE
HOT SPOT OF THE TF-COIL FOR A ONE AND
TWO-DIMENSIONAL ANALYSIS

	Response Uncertainties, $\Delta R/R$, in Percent for the Copper d.p.a. in the TF-Coil	
	One-Dimensional Analysis	Two-Dimensional Analysis
All Cr due to XS-Uncertainty	52.70	27.80
due to SED-Uncertainty	3.33	3.54
All Fe due to XS-Uncertainty	44.68	43.00
due to SED-Uncertainty	13.71	10.55
All Ni due to XS-Uncertainty	15.88	11.81
due to SED-Uncertainty	1.36	2.44
All Cu due to XS-Uncertainty	6.30	6.05
due to SED-Uncertainty	5.03	3.81
All C due to XS-Uncertainty	4.05	3.58
due to SED-Uncertainty	0.65	0.16
All H due to XS-Uncertainty	1.89	1.81
due to SED-Uncertainty	---	---
All O due to XS-Uncertainty	---	---
due to SED-Uncertainty	0.47	1.21
Total ^a	73%	54%

^a Quadratic sums.

V. CONCLUSIONS

The two-dimensional sensitivity and uncertainty analysis code SENSIT-2D was applied to calculate uncertainties in the heating and copper d.p.a. in the TF coil of a FED conceptual blanket-shield design. Results from a two-dimensional analysis are generally in agreement with those resulting from a one-dimensional calculation. The largest uncertainties were caused by uncertainties in the chromium and iron cross sections. A re-evaluation of the covariance data for chromium might lead to smaller predicted uncertainties, and is strongly recommended.

VI. REFERENCES

1. M. J. EMBRECHTS, "Two-Dimensional Cross-Section Sensitivity and Uncertainty Analysis for Fusion Reactor Blankets," Los Alamos National Laboratory report LA-9232-T (1982).
2. M. J. EMBRECHTS, "SENSIT-2D: A Two-Dimensional Cross-Section Sensitivity and Uncertainty Analysis Code," Los Alamos National Laboratory report LA-9515-MS (1982).
3. T. J. SEED, "TRIDENT-CTR User's Manual," Los Alamos Scientific Laboratory report LA-7835-M (1979).
4. R. L. CHILDS, D. E. BARTINE, and W. W. ENGLE, Jr., "Perturbation Theory and Sensitivity Analysis for Two-Dimensional Shielding Calculations," Trans. Am. Nucl. Soc., **21**, 543 (1975).
5. 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).
6. S. A. W. GERSTL, D. J. DUDZIAK, and D. W. MUIR, "Cross-Section Sensitivity and Uncertainty Analysis with Application to a Fusion Reactor," Nuc. Sci. Eng., **62**, 137 (1977).
7. D. J. DUDZIAK, "Cross-Section Sensitivity and Uncertainty Analysis for Fusion Reactors (a Review)," Proc. of the Advisory Group Meeting on Nuclear Data for Fusion Reactor Technology, IAEA-A-TECDOC-223, IAEA, Vienna, Austria, 11-15 December 1978.
8. M. Z. YOUSSEF, R. W. CONN, and C. W. MAYNARD, "Impact of Cross-section Uncertainties on the Nuclear Design of Hybrid Reactors," Nuclear Technology/Fusion, **2**, 648 (1982).
9. S. A. W. GERSTL, "Sensitivity Profile for Secondary Energy and Angular Distributions," Proc. Fifth Int. Conf. Reactor Shielding, 18-23 April 1977, Knoxville, TN, Science Press, Princeton 1978.
10. 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, ORNL/RSIC-42 (1979).
11. C. I. BAXMAN and P. G. YOUNG (Eds.), "Applied Nuclear Data Research and Development, April 1 - June 30, 1977," Los Alamos Scientific Laboratory report LA-6971-PR, (1977).
12. M. J. EMBRECHTS, "Is a Third-Order Spherical Harmonics Expansion of the Flux Adequate for a Two-Dimensional Sensitivity Analysis for Fusion Reactor Blankets?," Los Alamos National Laboratory report LA-UR-81-616 (1981).
13. B. G. CARLSON, "Tables of Symmetric Equal Weight Quadrature EQ_n Over the Unit Sphere," Los Alamos Scientific Laboratory report LA-4734 (1971).
14. 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).
15. B. A. CLARK, "TRIDENT-CTR Cross Sections," Los Alamos National Laboratory Memorandum T-1-82-TCD-3 (1982).
16. 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).