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A One- and Two-Dimensional Cross-Section Sensitivity and Uncertainty Path of the AARE Modular Code System

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ABSTRACT

AARE, a code package to perform Advanced Analysis for Reactor Engineering, is a linked modular system for fission reactor core and shielding, as well as fusion blanket, analysis. Its cross-section sensitivity and uncertainty path presently includes the cross-section processing and reformatting code TRAMIX, cross-section homogenization and library reformatting code MIXIT, the 1-dimensional transport code ONEDANT, the 2-dimensional transport code TRISM, and the 1- and 2-dimensional cross-section sensitivity and uncertainty code SENSIBL. In the present work, a short description of the whole AARE system is given, followed by a detailed description of the cross-section sensitivity and uncertainty path.

INTRODUCTION

The AARE modular code system[1] is being developed jointly by the Paul Scherrer Institute (PSI) and the Los Alamos National Laboratory (LANL). It is based on the DANDE (Applied Nuclear Data, Core Neutronics and Depletion) code system[2] which was developed for analyses of advanced Liquid Metal Fast Breeder Reactor (LMFBR) concepts. In comparison to DANDE, AARE can be used for wider range of reactor lattice cell, whole reactor, shielding, and fusion blanket analyses. It includes additionally, the cross-section sensitivity and uncertainty and general purpose modules. Its general description is given in reference 1. As with DANDE, the data is transferred between the codes using CCCC[3] and CCCC-like[4] files. This minimizes the user's input, (and sources of errors) as well as input inconsistencies in the sequence of code calls.

The cross-section sensitivity and uncertainty path is based on that reported at IAEA Advisory Group Meeting on Nuclear Data for Fusion Technology in Gaussig, G D R [5] Since this meeting the CCCC-like TRISM[6] geometry file, GEOMTY, was incorporated into SENSIBL. The incorporation of the ONEDANT[4] geometry file, GEODST and the CCCC files NDXSRF and ZNATDN is under way. This will lead to a considerable reduction of user input to SENSIBL.

THE AARE SYSTEM

Currently AARE consists of five modules: applied nuclear data, neutronics, material depletion, sensitivity and a general purpose module. The thermohydraulics module is under preparation. A block diagram is given in Figure 1.

The Nuclear Data Module consists of the cross section shielding, coupling and reformatting program TRAMIX,[1] a PSI update of the TRANSX CTR code[7] and the cross section data li-

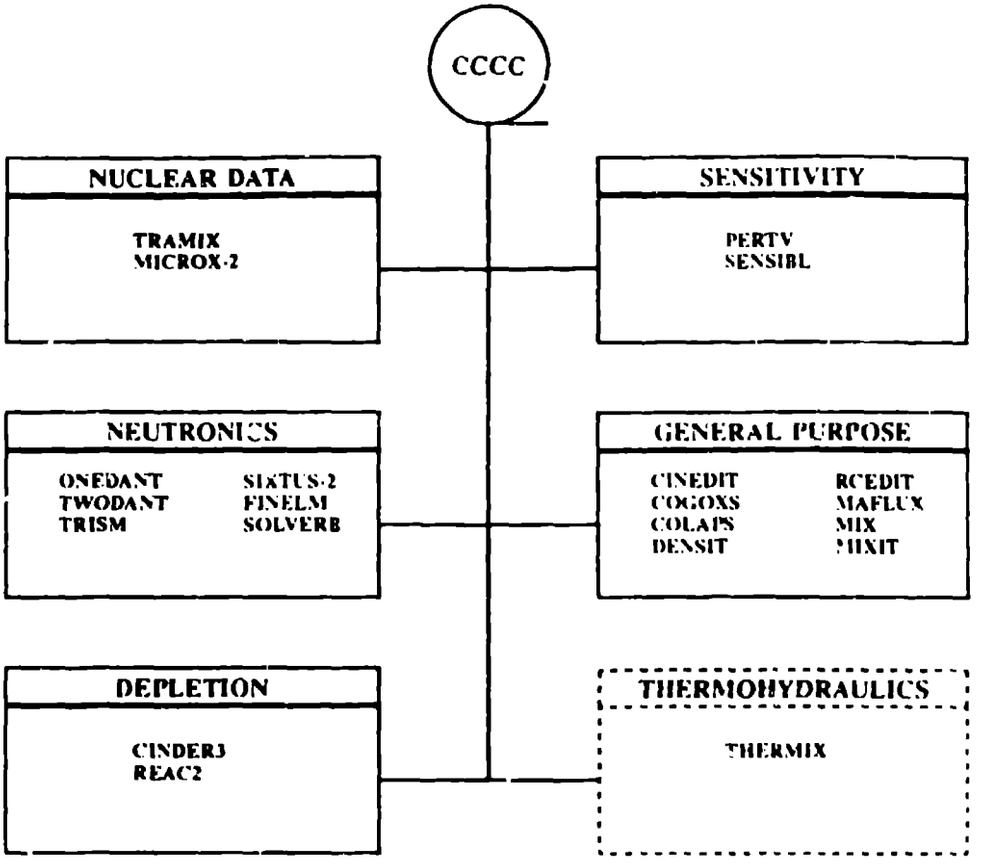

Figure 1. Block Diagram of the AARE System

The codes currently being used in the **Neutronics Module** include ONEDANT,[4] a one dimensional finite difference S_N transport code for slab, spherical and cylindrical geometries; TWODANT,[9] a two-dimensional finite difference S_N transport code, for x-y, r-z and r-θ geometries; TRISM,[6] a two-dimensional finite element S_N transport code for x-y, r-θ and toroidal geometries using triangular elements; FINELM,[10] a three-dimensional finite element diffusion code for x-y, r-z, r-θ, x-y-z and r-θ-z geometries using triangular or rectangular elements and SIXTUS-2,[11] a 2-dimensional nodal diffusion code for hexagonal geometry. A 3 dimensional hexagonal-z version is currently in preparation.

In addition to the aforementioned codes, the code SOLVERB, based on the coupled P_N/B_N method,[12] was included in the neutronics module. Eigenvalue, k_{eff} or buckling searches can be performed.

The **Depletion Module** presently consists of CINDER 3[2] with PSI updates, and REAC 2.[13] The CINDER-3 code is an enhanced version of CINDER 2. It uses explicit cross sections from the ISOTXS or GOXS file produced by TRAMIX, its own non explicit cross section file AFEW, and the RZFLUX file produced by the core neutronics module. A total of 233 products and 46 actinides in 186 chains are currently used in the CINDER 3 calculation.

For detailed material activation and transmutation calculations of fusion reactors, the depletion module REAC 2 was included into the system. This code presently uses the ENDF/B-V cross section library of over 300 isotopes and 6500 reactions. All materials between Z = 1 and 83

transmutation calculations without reverting to chaining specifications.

The **Sensitivity Module** presently consists of the two-dimensional perturbation theory code PERTV[14] and the one- and two-dimensional cross-section sensitivity and uncertainty analysis code SENSIBL.

PERTV is a two-dimensional perturbation theory code. It computes reactivity coefficient traverses using first-order perturbation theory, effective delayed neutron fraction, neutron generation time, the inhour/δ_k conversion factor and activity traverses. SENSIBL, an improved and accelerated version of SENSIT[15] and SENSIT-2D,[16] is a code based on first-order generalized pertubation theory.

At present eight codes are included in the **General Purpose Module**. They were designed to collapse and combine GOXS files, homogenize and/or print the cross-section sets from a GOXS file, to print and change isotopic densities on a ZNATDN file, and to print depletion history values etc. (See reference 1 for more details).

NUCLEAR DATA LIBRARIES

Four MATXS libraries based on the ENDF/B-V evaluations were generated at Los Alamos using the NJOY nuclear data processing system[17] and are only available within the USA. These are the 30n/12γ group MATXS5, 69n group MATXS7, 80n/124γ group MATXS6, and 187n/24γ group MATXS8 libraries described in reference 7.

Five additional libraries based on the Joint Evaluation File/European Fusion File (JEF/EFF) evaluations[18,19] were generated at PSI,[20,21] also using the NJOY nuclear data processing system.[17] These are the 70n group MAT70, 86n group MAT86, 175n/42γ group MAT175, 187n group MAT187, and 308n group MAT308 libraries. They are described in some detail in reference 1 also.

CROSS–SECTION SENSITIVITY AND UNCERTAINTY PATH

The cross-section sensitivity and uncertainty path consists at present of the codes TRAMIX, MIXIT, ONEDANT, TRISM and SENSIBL. The data linkage between these codes is primarily via CCCC and CCCC-like data files. Figure 2 displays the 1- and 2-dimensional flows.

TRAMIX uses the basic ENDF/B nuclear data in a fine-group MATXS library format,[7] generated from the NJOY code system.[17]

TRAMIX is able to shield resonance data in the whole energy range using the intermediate resonance absorption shielding method, (IR method),[22–24] by calculating energy- and isotope-dependent Goldstein-Cohen IR-factors and energy dependent Dancoff corrections. Using these, the effective background cross-sections can be calculated. This effective background cross section is then used together with temperature for interpolation in background cross-section and temperature dependent cross-section tables.[25] Both background cross sections and Dancoff corrections are calculated using the collision probability method. An extensive tabulation of the escape and transmission probabilities is used. For a more accurate interpolation, both are represented by arguments to their rational representation. Slab, spherical, cylindrical, pebble-bed, double heterogeneity grain, and cluster geometries are included. The method allows shielding of all zones in the system. Using the balance equation, the average fluxes are determined in all the regions, inclusive of the grains and their coatings. Using the rational expression for the flux, the background cross section is determined for each region of the spatial system.

The density-dependent IR method is based on the [illegible]

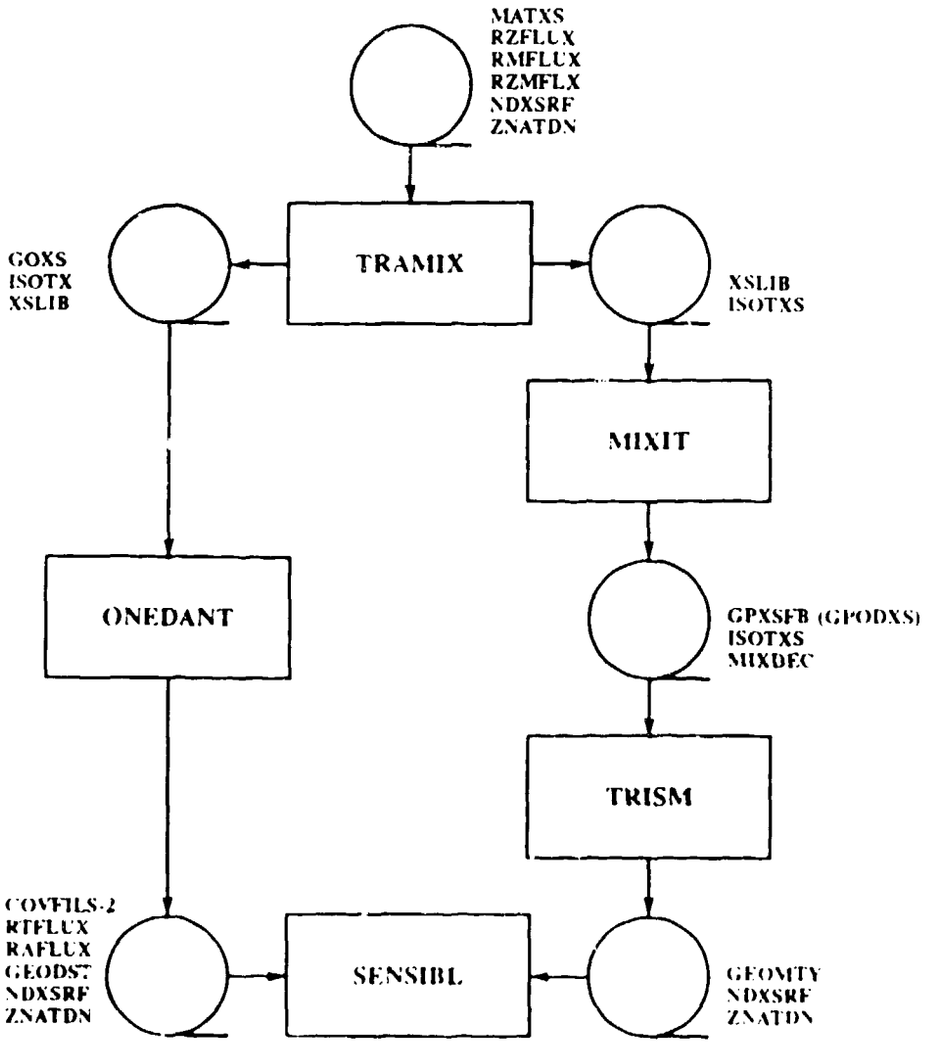

Figure 2. Flow Diagram of the AARE Cross-Section Sensitivity and Uncertainty Path

dent total and absorption multi-group cross-section tables.[1] Having those resonance parameters, the Goldstein-Cohen method[22,23] is used to calculate the IR-parameters.

In contrast to TRANSX-CTR, TRAMIX also reads the NDXSRF and ZNATDN files containing isotopic density specifications, which can override the input specifications. This is especially useful during a single run with multiple calls to TRAMIX, due to material depletion.

TRAMIX accurately computes fission spectra from fission matrices, corrects self scatter and the first outscatter terms of the elastic scattering matrices for differences between actual flux and library weighting flux and produces a variety of library formats which can be used in most transport and diffusion codes. Additionally, the code contains options for adjoint tables, mixtures, Doppler corrections, group collapsing, cell homogenization, thermal upscatter, prompt or steady state fission, transport corrections and flexible response function edits.

MIXIT[6] is used to prepare mixed, macroscopic cross section libraries in either BCD or group-ordered binary formats for use in transport code calculations. The BCD format is that of the XSLIB cross section libraries as used in ONEDANT, TWODANT and TRISM. The group ordered binary form is that of the GPODXS library used in TRISM. [illegible]

either BCD card images, or from the CCCC standard binary interface file ISOTXS. MIXIT can also be used to combine BCD and ISOTXS input files into a single, and therefore much smaller, problem-dependent input file.

TRISM is a computer program for solving the two-dimensional neutral particle transport equation in rectangular (x-y) and cylindrical (r-z) geometries within a general domain having curved or other non-orthogonal boundaries. The spatial discretization is accomplished using triangular finite elements and discontinuous linear trial functions. TRISM is a follow-on version of TRIDENT-CTR[26] which includes deterministic streaming capabilities.[27] The use of this deterministic streaming option is useful in mitigating the inaccuracies due to the "ray-effect" which plague calculations for fusion systems with large internal void regions. The use of triangles in r-z geometry allows a user to accurately follow curved or irregularly shaped boundaries and material interfaces of toroidal and other fusion system shapes. TRISM maintains all of the capabilities of TRIDENT-CTR but incorporates a completely new user-friendly, free-field input format similar to that of ONEDANT[4] and TWODANT.[9] In addition, several new input and edit options have been added.

SENSIBL is a code based on first-order generalized pertubation theory. It has the capability for cross-section sensitivity and uncertainty analysis, secondary-energy-distribution (SED) sensitivity and uncertainty analysis, and design sensitivity analysis. The code allows slab, spherical, cylindrical, x-y or r-θ geometries and accepts group-dependent quadrature sets.

Presently, SENSIBL is intended for use with ONEDANT and TRISM. The triangular mesh used by TRISM allows unique modelling capabilities that are applicable to fusion reactor configurations, and thus SENSIBL can also analyze these configurations. The forward and adjoint angular fluxes calculated by ONEDANT and TRISM are required input to SENSIBL. 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.

To date the special geometry file, GEOMTY, generated by TRISM has been incorporated as an input to SENSIBL. This eliminates most of the user generated input to the code. Due to the triangluar meshes used in TRISM, GEOMTY is not strictly a CCCC file. The 1-dimensional geometry file, GEODST, output from ONEDANT, together with the CCCC files NDXSRF and ZNATDN, containing density data, will soon be incorporated into SENSIBL, thus eliminating further the explicit user input.

The theoretical backgrounds are given in references 5 and 16. The code allows the calculation of the uncertainties of simple, as well as complex, responses such as kerma, displacements per atom (dpa), activation rates, or tritium breeding. The calculation is based on the calculation of sensitivity profiles in connection with covariance data:

$$\left[\frac{\Delta I}{I}\right]^2 = \sum_{all\ xmg} \sum_{all\ x'm'g'} P^g_{xm} P^{g'}_{x'm'} \frac{\mathrm{cov}(\sigma^g_{xm}, \sigma^{g'}_{x'm'})}{\sigma^g_{xm}\sigma^{g'}_{x'm'}} \qquad (1)$$

In this expression σ^g_{xm} represents the interaction cross section for reactions of type x in material m in energy group g, $\mathrm{cov}(\sigma^g_{xm}, \sigma^{g'}_{x'm'})$ is the covariance matrix for the indicated multigroup cross-sections, and P^g_{xm} is the relative sensitivity profile of response I for cross section σ^g_{xm}, defined by

$$P^g_{xm} = \frac{\partial I/I}{\partial \sigma^g_{xm}/\sigma^g_{xm}} \qquad (2)$$

The relative sensitivity profile clearly can be interpreted as the fractional change in the response per fractional cross section change. Note that in Eq. (1) the first two factors in each [illegible]

The sensitivity profile for the response I can be expressed as

$$P^g_{xm} = \frac{1}{I}\left\{ R^g_{xm}\,\varphi^g_m - \sigma^g_{xm}\,\chi^g_m + \sum_{\ell=0}^{LMAX}\sum_{g'=g}^{IGM} \sigma^{g\to g'}_{xm\ell}\,\psi^{gg'}_{m\ell}\right\}, \tag{3}$$

The integral of the response over the volume of the "detector" (which may be the entire system) is

$$I = \sum_{i\ \epsilon\ det} V_i \sum_{all\ g} \phi^{0g}_{0i} \sum_{all\ xm} N_{mi}\,R^g_{xm}, \tag{4}$$

where V_i is the volume of spatial interval i, ϕ^{0g}_{0i} is the scalar flux in group g in interval i, and N_{mi} is the local atomic density of material m in interval i. The quantity R^g_{xm} appearing in Eqs. (3) and (4) is the "response function," a response-weighted microscopic cross-section. If the response of interest is the number of nuclear reactions of type x, then R^g_{xm} is just the microscopic cross-section for that reaction. However, if the response of interest is the total nuclear heating, for example, then R^g_{xm} is the partial kerma factor (in units of eV-barns) for reaction x in material m in group g. Other complex responses, such as dpa and total helium production, can also be accommodated using suitable definitions of R^g_{xm}.

The quantities φ^g_m, χ^g_m, and $\psi^{gg'}_{m\ell}$ appearing in Eq. (3) are atom density-weighted, spatial integrals of the flux defined in reference 5.

The first term in the brackets of Eq. (3) is the direct term.[28] Note that this term is non-zero only if reaction x in material m contributes to the detector response function, so that both R^g_{xm} and φ^g_m are non-zero.

The second and the third terms of Eq. (3) comprise the indirect term. These terms are called the "loss" term and the "gain" term, respectively. Note that the indirect term receives contributions only from intervals in which the density N_{mi} is non-zero. The indirect term may be derived from the expression for the forward difference approximation, Eq. (36) in reference 29 or Eq. (17) in reference 30 or Eq. (26) in reference 31, considering a two-dimensonal geometry and expansion of the scattering into Legendre polynomial series and the flux angular expansions into the series of spherical harmonics.

Presently the MATXS8[7] coupled 187-neutron/24-photon-group library based on ENDF/B-5, the MAT187[20,21] a 187-neutron-group library based on JEF-1/EFF evaluations and COVFILS-2,[32] the cross-section and covariance library, are used for cross-section sensitivity and uncertainty calculations with the AARE system. Whereas the MATXS8 and MAT187 libraries are used as input libraries for TRAMIX for transport calculations with ONEDANT and after collapsing, with TRISM, the COVFILS-2 library is the input library for SENSIBL and is used for cross-section sensitivity and uncertainty calculations.

The 74-neutron-group boundaries of COVFILS-2 library are included in the 187-group structure of MATXS8 and MAT187 libraries. This enables more accurate 1-dimensional 187 neutron group calculations with ONEDANT and, after collapsing into 74 neutron-group structure, with TRISM and SENSIBL. The 187-neutron-group libraries can be also directly collapsed in TRAMIX using the library neutron-weighting spectrum or a known, (generated in a previous calculation) neutron flux file such as RZMFLX or RMFLUX for example.

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