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THE SHIELDING FACTOR METHOD FOR PRODUCING EFFECTIVE CROSS SECTIONS: MINX/SPHINX AND THE CCCC INTERFACE SYSTEM

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ABSTRACT

The Shielding Factor Method is an economical designer-oriented method for producing the coarse-group space and energy self-shielded cross sections needed for reactor-core analysis. Extensive experience with the ETOX/1DX and ENDRUN/TDOWN systems has made the SFM the method of choice for most US fast-reactor design activities. The MINX/SPHINX system was designed to expand upon the capabilities of the older SFM codes and to incorporate the new standard interfaces for fast reactor cross sections specified by the Committee for Computer Code Coordination. MINX is the cross-section processor. It generates multigroup cross sections, shielding factors, and group-to-group transfer matrices from ENDF/B-IV and writes them out as CCCC ISOTXS and BRKOXS files. It features detailed pointwise resonance reconstruction, accurate Doppler broadening, and an efficient treatment of anisotropic scattering. SPHINX is the space-and-energy shielding code. It uses specific mixture and geometry information together with equivalence principles to construct shielded macroscopic multigroup cross sections in as many as 240 groups. It then makes a flux calculation by diffusion or transport methods and collapses to an appropriate set of cell-averaged coarse-group effective cross sections. The integration of MINX and SPHINX with the CCCC interface system provides an efficient, accurate, and convenient system for producing effective cross sections for use in fast-reactor problems. The system has also proved useful in shielding and CTR applications.

INTRODUCTION

The complexity of a typical reactor core makes it impractical to solve the neutron transport problem with full space and energy detail. For this reason designers normally use effective cross sections averaged over relatively coarse energy groups and space regions. The Shielding Factor Method (SFM) is an economical method for producing these effective cross section that was originally developed in Russia.[1] Development of the SFM in the US has been chiefly for the fast-reactor program, and extensive experience has been accumulated with the ETOX[2]/1DX[3] and ENDRUN[4]/TDOWN[5] code systems. More recently the SFM has received increased attention for thermal power reactor analysis with the development of EPRI-CELL and EPRI-CPM for the electric utility industry.[6] SFM code systems are traditionally divided into two parts: the cross section processor (e.g., ETOX) and the space-energy collapse code (e.g., 1DX). The MINX/SPHINX system follows this pattern. It was designed to expand upon the capabilities of the older SFM codes and to incorporate the standard interface formats for fast reactor codes specified by the Committee for Computer Code Coordination (CCCC).[7] The MINX[8] cross section processor generates a library of multigroup cross sections, shielding factors, and group-to-group transfer matrices from ENDF/B-IV[9] evaluated nuclear data and writes it out as CCCC ISOTXS and BRKOXS files. The SPHINX[10] space-energy code uses specific mixture and geometry information together with equivalence principles and a diffusion or transport flux calculation to construct effective coarse-group cell-averaged macroscopic cross sections in CCCC format.

The MINX/SPHINX system is in routine use on both IBM and CDC equipment. Comparisons with the older SFM codes show generally good agreement. Comparisons with independent codes such as ETOE-2[11]/MC^2-2,[12] VIM,[13] and GGC-5[14] give confidence that the MINX/SPHINX system is suitable for the routine analysis of large fast-reactor cores.

THEORY OF THE SHIELDING FACTOR METHOD

The goal of the SFM is to define effective cross sections for some range of energy (E in group g) and some region of space ($\underline{r}$ in volume v) that preserve macroscopic overservables such as reaction rate. Clearly,

$$\sigma^i_{xgv} = \frac{\int_g dE \int_v d\underline{r}\ \sigma^i_x(E,\underline{r})\ \phi\ (E,\underline{r})}{\int_g dE \int_v d\underline{r}\ \phi\ (E,\underline{r})}\ , \tag{1}$$

where σ^i_x is the cross section for isotope i and reaction x at E and $\underline{r}$, and ϕ is the neutron scalar flux at that energy and position. Similar expressions can be constructed to preserve the group-to-group scattering rates and the transport cross section.

Unfortunately, the flux needed for Eq. (1) is not known before the fact; in fact, it is one of the quantities being sought in the analysis. In addition it is very complex, being full of sharp dips and peaks caused by resonances in the cross sections. However, experience has shown that it is possible to separate the variation of the flux into a part that is relatively smooth with respect to energy group and spatial zone size and a remaining resonance part. The variations in the smooth part can be determined by a multigroup flux calculation, but the intra-group flux must be selected by model.

The class of codes represented by MC^2 and GGC-5 determines this model flux by making a detailed flux calculation for a simplified homogeneous system. This is an expensive procedure. The SFM codes, on the other hand, assume that the intragroup flux can be modeled as

$$\phi(E) = \frac{W(E)}{\Sigma_t(E)} \quad , \tag{2}$$

where W is a smooth function of energy reflecting the fission and scattering sources into E and Σ_t is the total macroscopic cross section. Formally, Eq. (2) gives the flux for an infinite homogeneous system satisfying the narrow resonance approximation. However, heterogeneous systems can be included using equivalence princples.[15] Extension to wide and intermediate-width resonances is also possible.[16]

Furthermore, in evaluating the numerator of Eq. (1), it is assumed that the important effect is the interaction between a resonance in σ_x and the dip in the flux caused by that resonance (self-shielding). The reaction rate becomes

$$\int_g \frac{\sigma_x^i(E)}{\sigma_0^i + \sigma_t^i(E)} \, W(E)dE \tag{3}$$

where

$$\sigma_0^i = \frac{1}{\rho_i} \sum_{j \neq i} \rho_j \sigma_t^j \quad , \tag{4}$$

and where ρ_i is the number density for isotope i in the homogeneous mixture. The simplification comes from assuming that σ_0 is constant in g. The result is a single parameter, the "background cross section per atom," which can be used to characterize self-shielding. The cross sections produced by MINX are computed using

$$\sigma_{xg}^{i} = \frac{\int_g \frac{\sigma_x^i}{\sigma_0 + \sigma_t^i} W dE}{\int_g \frac{1}{\sigma_0 + \sigma_t^i} W dE} . \tag{5}$$

The results are tabulated as cross sections for $\sigma_0 = \infty$ and shielding

$$f_{xg}^{i} = \frac{\sigma_{xg}^{i}(\sigma_0)}{\sigma_{xg}^{i}(\infty)} , \tag{6}$$

for several values of σ_0. SPHINX then computes σ_0^i using Eq. (4). In heterogeneous systems an additional "escape cross section per atom" is added. The corresponding shielded cross section is then obtained by interpolating the f-factors for this σ_0. Temperature is handled in the same way.

This approach makes a composition-independent cross-section library possible. The economy of the SFM results from being able to use this library many times.

THE MINX PROCESSING CODE

MINX was designed to combine and improve upon the resonance capabilities of ETOX[2] and ENDRUN[4] and the anisotropic scattering capabilities of ETOG[17] and SUPERTOG.[18] It is a modular code that uses paging techniques and variable dimensioning to make it possible to process the complex evaluations found in ENDF/B-IV.9 The normal flow through the code is pictured in Fig. 1.

First, detailed pointwise cross sections are generated from ENDF/B resonance parameters and cross sections using the method of RESEND.[19] The energy grid is suitable for linear interpolation to within a user specified accuracy. The results are written out as a "pointwise-ENDF" (PENDF) tape suitable for printing, plotting, or further processing.

These pointwise cross sections are then accurately Doppler broadened to any desired temperatures using the method of SIGMA-1.[20] This approach has the advantage of correctly broadening smooth cross sections, backgrounds, and multi-level representations. Since broadening is a smoothing process, the results are thinned to a user specified accuracy and written out as PENDF tapes. Examples of the number of points produced in reconstruction and Doppler thinning are given in Table 1. Although this highly accurate process is expensive, it only has to be done once for a particular evaluation. Many subsequent averaging runs with different parameters can be made using the one temperature-dependent PENDF

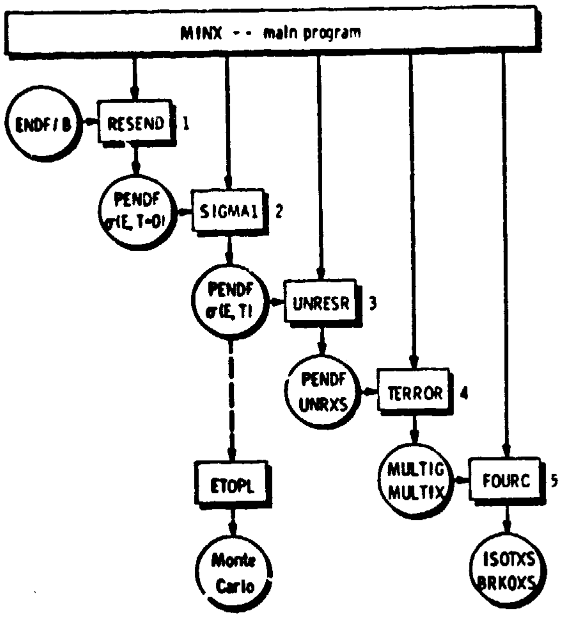

Fig. 1. Structure of MINX code illustrating functional blocks and data flow. ETOPL is not a part of MINX.

Table 1. Results of MINX Resonance Reconstruction and Doppler Broadening

Nuclide	Points at 0 K[a]	Points at 2100 K[b]	CP Seconds (CDC7600)
^{12}C	404	404	68.1
Fe	8798	5033	302.8
^{235}U	7209	2660	492.3
^{238}U	50372	6683	3483

[a] 0.5% reconstruction except 1.0% for ^{238}U.
[b] 0.1% thinning tolerance.

tape. The tape can also be reworked for use by continuous-energy Monte Carlo codes.[21]

This procedure will not work in the unresolved energy range where only statistical knowledge of the resonances is available. Effective pointwise cross sections vs T and σ_0 are produced by averaging over the ENDF/B distributions of resonance widths using methods based on ETOX.[2]

Multigroup cross sections are computed using Eq. (5) and appropriate generalizations. The group structure and smooth weight function are chosen by the user. The energy integrations are performed by adaptive quadrature starting from the union grid of the functions in the integrands. The nature of the PENDF cross section grid assures that all features are well-represented. Fission yields are averaged to preserve $\nu\sigma_f$ and slowing-down parameters are averaged to preserve $\bar{\mu}\sigma_e$ and $\xi\sigma_e$. The transport cross section is computed as $\sigma_t - \bar{\mu}\sigma_e$ where "current" weighting is used for the total cross section.

Elastic and discrete-inelastic scattering both obey two-body kinematics. MINX usually performs the resulting complex integrals over energy and angle with a semi-analytic method[22] based on an expansion in the laboratory system. The analytic integrals are obtained by a recursion relation, and the single energy integral is performed adaptively to a user specified tolerance. When this is not appropriate (e.g., light isotopes and near thresholds) MINX automatically changes to a direct numerical integration in the center-of-mass frame.

Group-to-group cross sections for continuum reactions are evaluated using analytic integrations over secondary energy and the standard adaptive quadrature for initial energy. Fission chi vectors by isotope are produced by averaging the ENDF/B spectrum appropriate to a specified incident energy.

The final step is to format the results of the multigroup averaging module into the CCCC-III[7] ISOTXS (cross sections and matrices) and BRKOXS (shielding factors) files.

THE SPHINX SPACE-ENERGY CODE

SPHINX combines an extended version of the resonance treatment of 1DX[9] with the one-dimensional diffusion theory flux calculation of 1DX or the one-dimensional transport flux transport of ANISN.[23] It is modular in structure and uses the flexible POINTR system[24] of dynamic storage allocation. The entire code was assembled in accordance with the CCCC specifications for code compatibility.[7,25] The use of CCCC interface files makes communication with other CCCC-compatible codes such as TWOTRAN[26] and VENTURE[27] straightforward.

The basic structure of SPHINX is shown in Fig. 2. The various execution paths through the code are administered by the ZEUS CONTROL module using input data from the CCCC standard and code-dependent interfaces listed in Table 2. The fundamental cross-section data, intermediate results, and final answers are transmitted using the CCCC files described in Table 3.

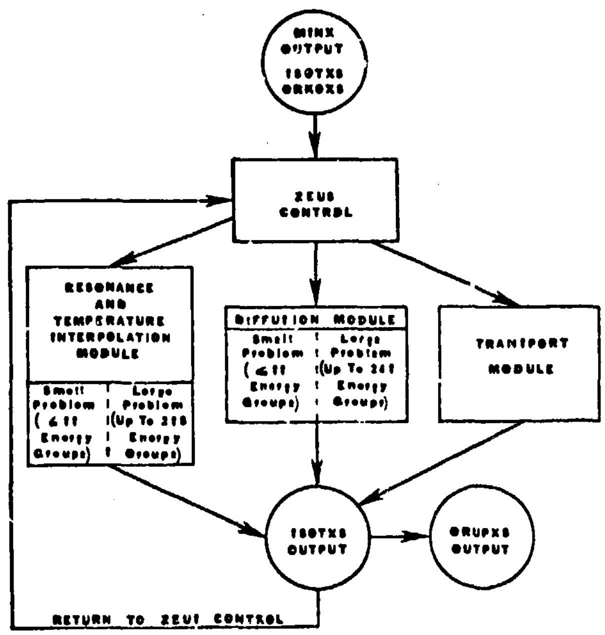

Fig. 2. Execution paths through SPHINX.

Table 2. SPHINX Control Files

Name	Standard	Description
ZEUS1A	no[a]	Modular control input
XSRINP	no	Resonance module input
SKODXI	no	Diffusion module input
ANISIN	no	Transport module input
ZNBTDN	no	Zone atomic densities
FPRINT	no	Print control
GEODST	yes[b]	Geometry description
NDXSRF	yes	Nuclide density and cross section parameters
ZNATON	yes	Zone nuclide atomic densities
SEARCH	yes	Criticality search parameters
SNCONS	yes	S_n constants
FIXSRC	yes	Volume and surface sources

[a]See Ref. 10 for detailed specifications.

[b]See Ref. 7 for detailed specifications.

Table 3. SPHINX Standard[a] Interface Files

Name	Description
ISOTXS	Nuclide-ordered cross section data
GRUPXS	Group-ordered cross section data
BRKOXS	Resonance self-shielding data
RTFLUX	Regular scalar flux
ATFLUX	Adjoint scalar flux
RCURNT	Regular current
ACURNT	Adjoint current
RAFLUX	Regular angular flux
AAFLUX	Adjoint angular flux
RZFLUX	Regular zone-averaged flux
PWDINT	Power densities

[a]See Ref. 7 for detailed specifications.

The first step in most problems is to use the resonance module to prepare effective self-shielded cross sections appropriate to the specified composition and geometry. The background cross section σ_0 is computed for each group and nuclide using Eq. (4). An additional escape term can be added for one of the seven options: (1) cylindrical cell using Sauer's approximation28 for the Dancoff factor in a hexagonal lattice, (2) cylindrical cell using Sauer's approximation to the Dancoff factor in a square lattice, (3) symmetric slab cell, (4) asymmetric slab cell, (5) isolated rod, (6) cylindrical cell with the Bell approximation[29] to the Dancoff factor, and (7) symmetric slab cell with the Bell approximation. Self-shielding factors are then computed at σ_0 by Langranian interpolation. Effective cross sections are defined as in 1DX except that provision is made for an elastic group-to-group matrix. The results are written in ISOTXS format for communication with the flux modules.

On option, the code then branches to the diffusion module. The calculation is identical to that in 1DX except that input is in ISOTXS format and cross-section storage has been modified to allow for up to 240 groups and for several additional partial reaction types (i.e, n2n, nα, nd, ...). The cross sections are then collapsed to a subset group structure using the computed flux and written out in ISOTXS format.

The optional transport module uses the S_n method to obtain the flux. The method is identical to ANISN except for the ISOTXS interface capability. When the flux has been obtained, cross sections are collapsed to a subset group structure and zone-averaged using either volume or flux weighting. This provides a capability for cell homogenization.

The use of standard files provides many possible paths. For example, the flux from a diffusion calculation is easily available as an input guess for a subsequent transport calculation using already shielded cross sections.

LIBRARIES AND UTILITIES

SPHINX is normally used with one of the existing multigroup libraries generated by MINX. LIB-IV[30] is a 50-group 101-isotope library generated from ENDF/B-IV. The library includes all the general purpose evaluations from ENDF/B-IV plus the two copper isotopes and the nine lumped fission products from ENDF/B-III. All materials were run at 300, 900, and 2100 K using 4 to 6 σ_0 values with decade steps. Scattering matrices are given to P_3. The weight function consists of a 1.4 MeV fission spectrum joined at 820.8 keV to a 1/E shape which, in turn, joins to a 0.025 eV Maxwellian at 0.10 eV. The library also contains delayed neutron yields and spectra for seven isotopes generated in CCCC DLAYXS format using NJOY.[31]

VITAMIN-C[32] is a 171-group library with 36 isotopes chosen for imfor temperature, σ_0, Legendre order, and weight function are similar to LIB-IV, except that a velocity exponential fusion peak has been attached in the 14 MeV range.

These libraries require several utility codes in order to knit them into a system with MINX and SPHINX. First, BINX[33] is a code for converting back-and-forth between binary and BCD modes for transmission of ISOTXS, BRKOXS, and DLAYXS files between laboratories. LINX[33] is a code for adding new isotopes to an existing CCCC cross-section library. Finally, CINX[34] is a collapse code that can be used to generate a subset library tailored to a particular set of problems. As an example, CINX has been used to produce a 126-group subset of VITAMIN-C especially designed for LMFBR core and shield analysis.[35] Figure 3 illustrates how these codes and libraries combine to form a complete system.

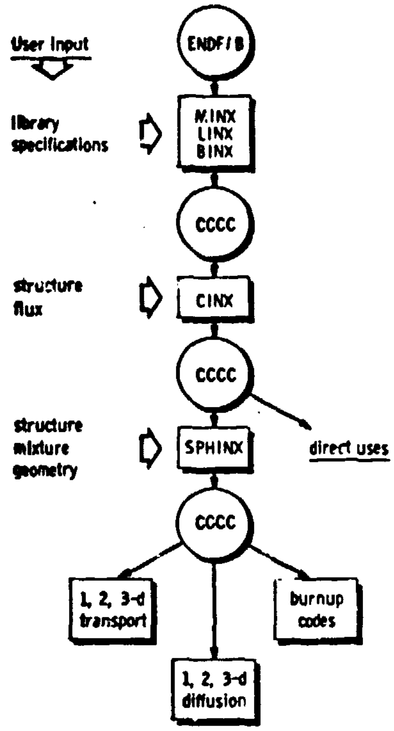

Fig. 3. Outline of CCCC interface system for generating multigroup constants for fast reactor analysis.

CODE VALIDATION

The MINX/SPHINX system has been tested in a variety of ways.[32-35] One ongoing project is a comparison of various processing codes being carried on by a committee of industrial and national laboratories (the DOE Code Evaluation Working Group). In order to minimize confusing complications, this group as analyzed a simple homogeneous composition typical of a large fast-breeder reactor core. The current results for some important parameters are given in Table 4. Larger differences exist between the fluxes and various cross sections. At the present time, for this type of problem, the chief causes of these differences seem to be: (1) group structure and weight function, (2) elastic removal treatment and (3) unresolved self-shielding. In any case, the numbers in Table 4 are less than the uncertainties associated with the basic evaluated data and with other design conservatisms. They imply that the MINX/SPHINX system is accurate for routine fast-reactor design.

Table 4. Comparison of Various Codes for a Buckled Homogeneous Fast Reactor Model

Parameter	ANL MC -2 Value	ARD 50 g/SPHINX % diff	ORNL 126 g/SPHINX % diff	LASL 50 g/1DX % diff	LASL ETOX/1DX % diff	GE 50 g/TDOWN % diff
k_{eff}	1.0040	0.10	0.31	0.19	0.13	0.17
C28/F49	0.1585	-0.06	-0.88	-0.26	-0.32	0.00
C28/F25	0.1447	-0.35	-0.76	-0.35	-0.48	0.28
F49/F25	0.9132	-0.33	0.12	-0.12	-0.23	0.22
F28/F25	0.0206	0.44	1.12	0.68	-0.44	4.27
F40/F25	0.1806	0.17	0.55	0.33	-0.44	1.55
F41/F25	1.294	0.29	0.36	0.33	-0.15	0.30

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