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Cross-Section Methodology in SIMMER

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ABSTRACT

The cross-section methodology incorporated in the SIMMER code is described. Data base for all cross sections is the ENDF/B system with various processing computer codes to group collapse and modify the group constants which are used in SIMMER. Either infinitely dilute cross sections or the Bondarenko formalism can be used in SIMMER. Presently only a microscopic treatment is considered, but preliminary macroscopic algorithms have been investigated.

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1. INTRODUCTION

Neutron cross-section implementation in the SIMMER¹ code is designed to meet four criteria: 1) availability, 2) economy, 3) flexibility, and 4) reliability. The Bondarenko formalism is an economical, yet reliable technique for generating temperature and self-shield cross sections. ENDF/B² data is employed in the generation of the self-shielding factors. A number of computer codes have been developed for group collapsing, format manipulations and updating.

All pointwise and fine group cross sections are obtained from ENDF/B-IV, with the exception of fission products which are ENDF/B-III, using the MIXX³ and XJOY⁴ processing codes. Output from these codes is input into CBXN,⁵ PCFTR,⁶ and FTRCOL⁷ for formatting changes, data manipulation and updating.

The few group infinitely dilute cross sections (ISOTXS⁷ file) and the self-shielding factors (BRKXS⁷ file) are read into SIMMER and stored in large core memory (LCM). This data is readily available for utilization in the determination of temperature and self-shielded cross sections.

A temperature-dependent k -factor (f) for a particular isotope at a given temperature is determined by a 3-point Lagrangian interpolation on the $(\ln T, f)$ tabular points. The background cross-section

(σ_0) interpolation employs a hyperbolic tangent dependence on $\ln \sigma_0$ for a given temperature.⁸

Shielded microscopic cross sections are calculated for each isotope (that has f -factors) at each mesh cell in the problem. The shielded microscopic cross sections are used to generate shielded macroscopic cross sections. Preliminary work has begun on the direct calculation of shielded macroscopic cross sections for each component in each mesh cell. This procedure will reduce the cross-section processing time.

II. CROSS-SECTION SOURCES

Although SIMMER uses broad group cross-section information, there are three preliminary steps before the broad group cross sections can be input to SIMMER. First, pointwise cross sections are generated from ENDF/B; second, fine group libraries are obtained and finally the fine group library is collapsed to the broad group library using appropriate weighting spectrum.

A. Fine Group Library

The data base for all cross-section information is the ENDF/B system. With the exception of the various combined fission products (i.e., rapidly saturating fission product produced by preceding nuclide, etc.), all nuclear data is obtained from

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END 8-11. The combined fission product information is obtained from EXMP/8-111. To process the EXMP/8 libraries, the computer codes MINX and XJOY are employed. Both MINX and XJOY produce pointwise cross-section information to within some specified tolerance for the resonance regions. Furthermore, these codes supplier broaden the pointwise cross sections to any number of specified temperatures. The pointwise supplier-broadened cross-section information is saved on tapes (called FEND tapes) such that, in the event at some later date additional temperatures are required, MINX and XJOY can start with the pointwise data. This saves significant computation time as the pointwise data does not have to be reconstructed.

Once the pointwise libraries have been generated, MINX/XJOY calculate the fine group constants (e.g., 50-group ISOXS and BRKXS standard interface files). Generally a 1/E plus a fission spectrum with a specified 1/E cutoff and nuclear temperature is employed as the energy weighting spectrum. There is no implicit spatial weighting in the generation of the fine group cross sections.

The shielding factors and infinitely dilute cross sections are the bulk of group constants which are required in SIMMER. There are other required group constants. A complete specification is given in Table 1 for the specific group constants which are required in SIMMER for the determination of self-shielded cross sections. Note that the resonance self-shielding factors are given for discrete E_0 and temperature values. This will be discussed in detail in Section IV.

Although MINX/XJOY output standard interface files (ISOXS and BRKXS), the files are not directly usable in the 10/75 version of SIMMER. Since the Bondarenko formalism is used, only the inelastic scattering matrices with (n,2n) modifications are required in SIMMER. These modifications and a few other minor modifications are performed by the CIXX or FCFTR code. CIXX/FCFTR also convert the fine group standard interface libraries to the FTR (10X) format which is the required format for the collapsing code FTRCOL.

B. Broad Group Library

As it is not economical to run the SIMMER code with a large number of energy groups (i.e., >10), the FTRCOL code has been developed to collapse the cross section and f-factors to some subset of the fine

TABLE 1

SPECIFIC GROUP CONSTANTS REQUIRED FOR SIMMER TO CALCULATE SELF-SHIELDED CROSS SECTIONS

Symbol	Name
σ_f	Infinitely dilute fission cross section
σ_c	Infinitely dilute capture cross section
σ_e	Infinitely dilute elastic cross section
σ_{in}	Infinitely dilute total inelastic scattering cross section (includes (n,2n) reaction)
σ_t	Infinitely dilute total cross section $\sigma_t = \sigma_f + \sigma_c + \sigma_e + \sigma_{in}$
ν	Average number of neutrons released per fission
μ	Average cosine of the elastic scattering angle
σ_d	Elastic slowing-down cross section
$\sigma_{tr}^{(1)}$	Inelastic transfer cross section from group 1 to group j (includes (n,2n) reaction)
$f_f(E_0, T)$	Total cross-section self-shielding factor
$f_e(E_0, T)$	Elastic cross-section self-shielding factor
$f_f(E_0, T)$	Fission cross-section self-shielding factor
$f_c(E_0, T)$	Capture cross-section self-shielding factor

group library. FTRCOL outputs the cross-section information in standard interface files (ISOXS and BRKXS); however, only the modified inelastic scattering matrix is included in the ISOXS file. Also, the elastic removal cross section in the BRKXS file has been corrected by the collapsing flux spectrum. It should also be pointed out that the f-factor has been collapsed via an infinite dilute type of spectrum. For more details one should see the FTRCOL report.

III. CROSS-SECTION UTILIZATION

Cross-section methodology in SIMMER consists of either self-shielded or infinitely dilute cross sections. As discussed earlier, if one desires shielded cross sections, the Bondarenko formalism is applied to the microscopic cross sections and macroscopic cross sections are determined. On the other

hand, if one employs infinitely dilute cross sections, either microscopic or macroscopic cross sections are permitted.

2. Input of Data

Cross-section information is input to SIMMER either via cards or tape/disk. Both methods of input are not permitted.

1. Card Input

Infinitely dilute cross sections, either microscopic or macroscopic can be entered by cards. The cross sections must be in the LASL format suitable for reading by the LASL block loader. Presently there is no option, nor is it advised to enter cross-section information suitable for use in the Bondarenko formalism by means of cards.

2. Tape/Disk Input

Only the ISOTXS and BRKOXS files are read by SIMMER if the tape input option is selected. Utilization of the ISOTXS information is straightforward with three exceptions. First, the group average velocities on the ISOTXS files are in cm/sec, thus a conversion is made to m/sec. Second, the inelastic scattering matrix must contain the inelastic scattering data with appropriate n, n modifications. Other scattering matrix data may be on the ISOTXS file, but will be ignored by the SIMMER code. Finally, the option of selecting the isotope chi vector to be used for the problem is available. This is the last entry in the ISO ID vector. The ISO ID vector specifies what isotope numbers are to be retrieved from the master broad group library; the ISO ID vector has MTPS (total number of isotopes used in the problem) entries. The MTPS+1 entry specifies what isotope is to be used in selecting a chi vector.

BRKOXS information implementation is direct with two exceptions. First, the transport self-shielding factors are not used in SIMMER. The total, capture, and elastic self-shielding factors are used to calculate the shielded transport cross section. Finally, there are six cross sections read from the BRKOXS file; however, only four of them are used. The potential scattering cross section and the average elastic scattering lethargy increment are not used in SIMMER. In their place the total and capture cross sections from the ISOTXS file are stored. Table II gives a list of the cross sections stored

TABLE II
STORAGE OF CROSS SECTIONS IN THE FXS ARRAY

Type	Name
1	P_0 weighted total cross section (Barns)
2	Capture cross section (Barns)
3	Inelastic cross section (Barns)
4	Elastic cross section (Barns)
5	Average cosine of elastic scattering angle
6	Elastic down-scattering to adjacent group

in the FXS cross-section array. These infinitely dilute cross sections are used in the calculation of the background cross sections as well as self-shielded cross sections.

The temperature-dependent f-factor (f) for a particular isotope at a temperature T is determined by a 3-point Lagrangian interpolation on the $(\ln T, f)$ tabular points. Rather than determine the interpolation coefficients every time they are needed for a cross section in a mesh cell, the coefficients are calculated at the input stage and stored for later use. This does not require any additional storage since the actual $f(T)$ values no longer need to be stored.

IV. SELF-SHIELDED CROSS SECTIONS

For a particular mesh cell in SIMMER there are NC components. Each of the components has a corresponding temperature and number density. At input time the isotopes which make up the components are specified. Accordingly sufficient information is available to determine temperature and self-shielded cross sections. Presently only a microscopic treatment has been thoroughly investigated and implemented in SIMMER. Preliminary work has begun on calculating self-shielded macroscopic cross sections. Although this work is not complete, it will afford a significant savings in cross-section processing time.

A. Microscopic Calculation

Having temperature, density, and isotope information for each mesh cell in SIMMER, it is straightforward to calculate shielded microscopic cross sections and in turn generate the required macroscopic cross sections for each mesh cell. The calculation of shielded cross sections is divided into four phases: 1) background cross-section

determination, 2) f-factor calculation, 3) calculating shielded microscopic cross sections, and 4) generation of cell macroscopic cross sections. The phases can be summarized by

$$\bar{\sigma} = f(\sigma_0, T) \sigma_0 \quad (1)$$

where $\bar{\sigma}$ = self-shielded cross section,

σ_0 = infinitely dilute cross section,

f = resonance self-shielding factor,

T = temperature,

σ_0 = background cross section.

Each of the terms in Eq. (1) has been defined in Table I. The f-factors are given for discrete values of σ_0 and T , as a consequence of the fine group constant generation. Table III indicates the format for storage of the f-factors; although the table depicts temperatures, recall that only the coefficients of the temperature fit are stored. In general f-factor information for three temperatures and five-to-six values of σ_0 are utilized in SIMMER.

1. Background Cross Section

The background cross section $\sigma_{0,j}$ is a parameter which represents the total macroscopic cross section due to all atoms (except the j'th) in a given mesh cell. In the Bondarenko scheme it is assumed to be constant in energy over the energy group interval. For the k'th cell we can say that the total macroscopic cross section for group g is

$$\sigma_t^g = N_j \sigma_{t,j}^g + \sum_{k \neq j} N_k \sigma_{t,k}^g \quad (2)$$

where N_i = number density for the i'th isotope,

σ_{ti}^g = total microscopic cross section for the i'th isotope.

TABLE III

STRUCTURE OF f-FACTOR STORAGE

Temperature (K/n)	Background Cross Section (σ_0^n)				
	1	2	3	4	5
T_1	$f_{11}(f_u)$	f_{12}	f_{13}	f_{14}	$f_{15}(f_\ell)$
T_2	f_{21}	f_{22}	f_{23}	f_{24}	f_{25}
T_3	f_{31}	f_{32}	f_{33}	f_{34}	f_{35}

$$\sigma_0^1 > \sigma_0^2 > \dots > \sigma_0^n; T_3 > T_2 > T_1$$

Dividing Eq. (2) by N_j we have

$$\frac{\sigma_t^g}{N_j} = \sigma_{t,j}^g + \frac{1}{N_j} \sum_{k \neq j} N_k \sigma_{t,k}^g \quad (3)$$

the second term on the right-hand side of Eq. (2) is the customary definition of the background $\sigma_{0,j}$. Thus one can see that σ_0 is an indication of the effect of other isotopes in a mix, especially in the vicinity of large cross-section resonances. Defining σ_0 as

$$\sigma_{0,j} = \frac{1}{N_j} \sum_{k \neq j} N_k \sigma_{t,k} \quad (4)$$

we see that $\sigma_{0,j}$ cannot be determined until the total cross section of all k isotopes is known. That is, since σ_t is a function of the correct f-factor, one must iterate to obtain both the shielding factors and the shielded total cross section. An initial guess for $\sigma_{0,j}$ in the g'th group is

$$1. \sigma_{0,j} = \frac{1}{N_j} \sum_{k \neq j} N_k \sigma_{t,k} \quad (5)$$

where $\sigma_{t,k}$ is the infinitely dilute total cross section. Subsequent σ_0 iterations (v) are given by

$$v+1. \sigma_{0,j} = \frac{1}{N_j} \sum_{k \neq j} N_k \left(\sigma_{c,k}^g \sigma_{e,k}^g + f_{t,k}^g \sigma_{t,k}^g + \sigma_{c,k}^g \sigma_{e,k}^g + \sigma_{in,k}^g \right) \quad (6)$$

where the terms in Eq. (6) have been defined in Table I. Furthermore, f^g is the f-factor which has been obtained by use of the σ_0^g value.

2. Self-Shielding Factor Calculation

Equation (6) indicates that for the determination of the background cross section one need calculate a self-shielding factor f . Since f is a tabular function of T and σ_0 it is necessary to perform an interpolation in the T and σ_0 space. The present algorithm is structured such that, given a T and a σ_0 , one can directly calculate the corresponding f-factor without additional interpolation. However, it is constructive to examine each interpolation procedure.

a. Temperature Interpolation

As discussed in Section III.A.2 the coefficient of a 3-point Lagrangian fit have been stored in lieu of the actual f-factor. Thus for temperature T' we have

$$f(T') = \alpha(\ln T')^2 + \beta \ln T' + \gamma \quad (7)$$

where α , β , γ are the predetermined coefficients and are available for each isotope.

b. Background Cross-Section Interpolation

In a recent paper,⁹ Kidman has shown that the actual f-factor behavior for numerous groups and isotopes possesses a hyperbolic tangent dependence on $\ln \sigma_0$ for a given temperature. Consequently, to calculate the f-factor for a particular composition σ_0 one has

$$f(\sigma_0) = A \tanh [B(\ln \sigma_0 + C)] + D \quad (8)$$

The amplitude and ordinate placement of the tanh curve are described by parameters A and D. Parameters B and C can be determined by utilizing two (σ_0^n, f) points near the given σ_0 value. Direct application of Eq. (8) is costly on the computer since literally millions of tanh and ln would have to be taken during any given calculation. Consequently Eq. (8) has been recast into another form. After considerable algebra one can show for a current σ_0 and T'

$$f(\sigma_0, T') = \frac{f_u(T')f_l^n + f_l^n}{\delta^u + \beta} \quad (9)$$

$$\text{where } \delta = \frac{f_n(T') - f_l(T')}{f_u(T') - f_n(T')} + \frac{f_u(T') - f_{n1}(T')}{f_{n1}(T') - f_l(T')}$$

$$\beta = \frac{f_u(T') - f_{n1}(T')}{f_{n1}(T') - f_l(T')}$$

$$\alpha = \frac{\ln(\sigma_0^n / \sigma_0^{n1})}{\ln(\sigma_0^n / \sigma_0^{n1})}$$

$n1$ and n = upper and lower table points for the current σ_0 value (i.e., σ_0 lies between tabular points σ_0^{n1} and σ_0^n and $\sigma_0^{n1} > \sigma_0^n$), and

u and l = upper and lower f tabular values at σ_0^u and σ_0^l .

Equation (9) is equivalent to Eq. (8), but is approximately 25% faster in computation time. Therefore Eq. (9) is used in the present SIMMER version. FORTRAN coding and description of the subroutine which performs the background calculation and the f-factor calculation are given in Appendix A.

3. Calculation of Shielded Microscopic Cross Sections

Once suitable f-factors have been calculated they are applied to the infinitely dilute cross sections as specified in Eq. (1). In more explicit terms, the shielded cross sections for the g 'th energy group in SIMMER are:

$$\bar{\sigma}_f = f_f \sigma_f \quad (10)$$

$$\bar{\sigma}_a = f_f \sigma_f + f_c \sigma_c - \left[\sum_h \sigma_{in}(g \rightarrow h) - \sigma_{in} \right] \quad (11)$$

$$\bar{\omega}_f = f_f \omega_f \quad (12)$$

$$\bar{\sigma}_{tr} = \left[f_t \sigma_t + (f_f \sigma_f + f_c \sigma_c + \sigma_{in}) \right] (1 - u) + f_f \sigma_f + f_c \sigma_c + \sigma_{in} \quad (13)$$

$$\bar{\sigma}_{g-1 \rightarrow g} = f \sigma_{d,g-1} + \sigma_{in,g-1 \rightarrow g} \quad (14)$$

$$\bar{\sigma}_{g-2 \rightarrow g} = \sigma_{in,g-2 \rightarrow g} \quad (15)$$

$$\bar{\sigma}_{g \rightarrow g} = \bar{\sigma}_{tr} - \left[\bar{\sigma}_a - \sum_{g \neq l} \bar{\sigma}(g \rightarrow h) \right] \quad (16)$$

These cross sections are determined for each isotope in a mesh cell and are used in the calculation of the shield macroscopic cross sections. A FORTRAN listing of the subroutine which calculates Eqs. (10)-(16) is given in Appendix B.

4. Macroscopic Cross-Section Calculation

Macroscopic cross sections for each mesh cell are determined in two steps. The first step

consists of mixing the isotopes to form microscopic component cross sections. This step is necessary since only the component densities are available for calculating the cell macroscopic cross sections. Once the component microscopic cross sections have been calculated, the appropriate macroscopic cross sections for a mesh cell are determined by suitable selection of component microscopic cross sections and component densities. The steps are more explicit in the discussion of Appendix C. After all the macroscopic cross-section types for a fixed group have been calculated for the i, j mesh cell they are stored in large core memory. After all mesh cells have been processed the macroscopic cross sections are transferred from LCM to a disk and the next energy group is processed. When all mesh cells and energy groups have been processed the disk is rewound and subsequent neutronic subroutines read the disk file.

5. Cross-Section Computation Time

A statistical timing study for a 4-group problem is given in Appendix D. The histograms in Appendix D indicate the relative time spent in various portions of the subroutines, namely SHLDXS, FFGEX, and CSCAL, which determine the shielded cross sections. The REL ADDRESS column of Appendix D corresponds to the relative address of FFGEX (Appendix A), CSCAL (Appendix B), and SHLDXS (Appendix C). From the results of Appendix D one can conclude that approximately 15% of the computation time is spent calculating macroscopic cross sections, 72% calculating background cross sections and self-shielding factors, 6% calculating shielded microscopic cross sections, and 6% for miscellaneous calculations and input/output.

B. Macroscopic Calculation

There are NC (generally 3) components permitted in SIMMER and the components, say fuel, stainless steel, and coolant, are comprised of several (12-20) isotopes. In processing microscopic cross sections one has to perform 4-7 times as many calculations as might be required if one could calculate self-shielded macroscopic cross sections directly. This section addresses the possibility of determining component f-factors thus permitting direct calculation of self-shielded macroscopic cross sections.

One can define a macroscopic cross section for the g 'th group as:

$$\Sigma_{xi}^c = \sum_{i \in C} N_i^* \sigma_{ix} \quad (17)$$

- where c = component of interest,
 x = cross-section type (fission, capture, etc.),
 σ_{ix} = self-shielded microscopic cross section of isotope i and type x ,
 $N_i^* = \rho_c \left(\frac{N_i}{\rho_o} \right)$
 $\left(\frac{N_i}{\rho_o} \right)$ = input number density for the i 'th isotope,
 ρ_o = initial density of the c component,
 ρ_c = current density of the c component.

Equation (17) can be recast as:

$$\Sigma_{xi}^c = F_x^c \sum_{i \in C} N_i^* \sigma_{ix} \quad (18)$$

where F_x^c = the component f factor and
 σ_x^* = infinitely dilute cross section.
 Thus

$$F_x^c(\rho_o^c, T) = \frac{\sum_{i \in C} N_i^* f_{ix}(\sigma_o^*, T) \sigma_{ix}}{\sum_{i \in C} N_i^* \sigma_{ix}} \quad (19)$$

for each component. The total macroscopic cross section for a mesh cell is then

$$\Sigma_{x,m} = \sum_{k \in M} \omega_k F_x^k(\sigma_o^k, T) \sum_{i \in C} \frac{N_i}{\rho_o} \sigma_{ix} \quad (20)$$

where the inner summation is performed at the input stage rather than in the cross-section processing stage. The background cross section for the c 'th component is then

$$\Sigma_o^c = \frac{\sum_{i \in C} \sum_{t,n} \omega_{t,n}}{\rho_c \sum_{i \in C} \left(\frac{N_i}{\rho_o} \right)} \quad (21)$$

The drawback to direct application of Eq. (19) is the over shielding of the macroscopic cross sections, yielding too low a steady state eigenvalue. In calculating F_X^C by use of Eq. (19) only tabular values of σ_o are employed; thus the self-shielding within the c'th component or among the various isotopes which make up the c'th component is not correct, namely underestimated. What is needed for Eq. (19) to be useful is a continuum of σ_o values for the various isotopes, yet arranged in some way such that one has tabular background cross sections for the components, thereby permitting interpolation within the component data as its density and temperature in a given mesh cell change.

A proposed algorithm for the selection of a component background cross section is

$$\sigma_o = \frac{\sum_i \left(\frac{Y_i}{\sum_j Y_j} \right) \sigma_o^i}{\sum_i \frac{Y_i}{\sum_j Y_j}} \quad (22)$$

where

$$\sigma_o = \left(\frac{1}{\sum_i Y_i} \right) \left[\sum_i \left(\frac{Y_i}{\sum_j Y_j} \right) \sigma_o^i + Y \right] \quad (23)$$

In the expression for the pseudo-isotopic background of Eq. (23), the quantity Y represents the total macroscopic cross sections for the other components of a mix which might be found in a mesh cell. A few possible choices for Y are:

- (1) Preselect values for Y, say 10, 100, 1000, 10000.
- (2) Use of initial data to describe the other components in an average cell, namely the isotopic number density and infinitely dilute total cross section.

Consider one example of choice (2) where fuel consists of Pu and ϕ , the coolant is Na, and steel is Fe. Then the background cross section for the fuel is

$$\sigma_o^{Pu} = \frac{1}{N^{Pu}} \left[N^{\phi} \sigma_t^{\phi} + \left(N^{Na} \sigma_t^{Na} + N^{Fe} \sigma_t^{Fe} \right) \right] \quad (24)$$

$$\sigma_o^{\phi} = \frac{1}{N^{\phi}} \left[N^{Pu} \sigma_t^{Pu} + Y \right] \quad (25)$$

where $Y \equiv N^{Na} \sigma_t^{Na} + N^{Fe} \sigma_t^{Fe}$ = the other components of the mix. Adding Eqs. (24) and (25) yields

$$N^{Pu} \sigma_o^{Pu} + N^{\phi} \sigma_o^{\phi} = \left[N^{\phi} \sigma_t^{\phi} + N^{Pu} \sigma_t^{Pu} + 2Y \right] \quad (26)$$

so that the background for the fuel component might be

$$\sigma_o^{fuel} = \frac{\left(N^{Pu} \sigma_o^{Pu} + N^{\phi} \sigma_o^{\phi} \right)}{\left(N^{Pu} + N^{\phi} \right)} \quad (27)$$

$$= \frac{\left(N^{\phi} \sigma_t^{\phi} + N^{Pu} \sigma_t^{Pu} + 2Y \right)}{\left(N^{Pu} + N^{\phi} \right)} \quad (28)$$

By utilization of Eq. (28), the various component background cross-section information can be calculated by varying the value of Y and using available input information. This is an area which requires further investigation.

IV. CONCLUSION

The cross-section methodology in the present version of SIMMER has been discussed. Although SIMMER uses broad group constants in the Bondarenko formalism, the initial data is ENDF/B. Fine group libraries are generated using MINX and NJOY. The fine group library is spectrum collapsed with some group constants being flux corrected. If one enters cross sections via cards, only the LASL loader format can be used to enter infinitely dilute cross sections; however, if cross sections are entered via tape/disk, the standard interface files ISOTKS and BRKOXS are utilized. Self-shielding factors are calculated and applied to each isotope in each mesh cell for the problem. This is a microscopic treatment that is computationally expensive; however, some investigative work has been performed in the area of self-shielded macroscopic cross sections.

V. ACKNOWLEDGMENTS

The author would like to thank LaRon Smith for several interesting discussions in the utilization and implementation of the Bondarenko formalism especially in the area of f-factor interpolation schemes.

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APPENDIX A

SUBROUTINE FFGEN

CALCULATION OF BACKGROUND CROSS SECTION AND f-FACTORS

Following is a listing of subroutine FFGEN which calculates background cross sections and f-factors. Which isotopes and components to process are specified in the argument of FFGEN. The names and contents of the argument arrays are given below.

Argument Name	Contents
COMNLS(NC)	Number of mix instructions for the j'th component
COMCOM(NC,MTPS)	Mix commands for the j'th component
NSIGN(MTPS)	Number of tabular σ_0 /isotope
TEMP(NC)	Temperature (K) of the j'th component
SIG(MSIG,MTPS)	Tabular σ_0 for each isotope
SIG0(MTPS)	Calculated σ_0 for each isotope for input density and temperature
FCF(SMSIGI,4,MTPS)	Coefficients of the temperature f-factor 3-point fit

Argument Name	Contents
FSS(4,MT,1)	Calculated f-factors
C(INH,MT)	Infinitely dilute cross section
G	Energy group
NC	Number of components
MSIG	Maximum number of tabular σ_0 permitted (6)
MS3	SMSIG
INH	Number of rows in the cross section set usually INH = 104 (number of groups)
MT	Total number of materials in problem
COMRHO(NC,MT)	Isotope number densities in each component
FXS(6,MTPS)	BROOKS cross-section information (see Table II)
MTX	MTPS (number of isotopes from tape)
	others
RHOC	The density of the j'th component

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SUBROUTINE FFGEN(COMNLS,COMCOM,NSIGN,TEMP,SIG,SIG0,FCF
1,FSS,C,G,NC,MSIG,MS3,INH,MT,COMRHO,FXS,MTX)
C
C THIS SUBROUTINE CALCULATES F-FACTORS GIVEN A SIGU MATRIX AND F-
C FACTORS
C
32 INTEGER G,COMNLS,COMCOM
32 DIMENSION COMNLS(1),COMCOM(NC,1),NSIGN(1),TEMP(1),SIG(MSIG,1)
1,SIG0(1),FCF(MS3,4,1),FSS(4,MT,1),C(INH,MT),COMRHO(NC,1),FXS(6,MTX
1,1)
C TEMP ADDITION TO SAVE DIVIDES
32 DIMENSION RCOMR(3,70)
32 COMMON/RPASS/RHOC(10)
PS02075 72
PS02075 73
PS02075 74
FFGEN 5
FFGEN 6
FFGEN 7
FFGEN 8
PS02075 75
PS02075 76
PS02075 77
PS02075 78
PS02075 79
PS02075 80
PS02075 81
PS02075 82
PS02075 83
PS02075 84
PS02075 85
PS02075 86
PS02075 87
PS02075 88
PS02075 89
PS02075 90
PS02075 91
PS02075 92
PS02075 93
PS02075 94
PS02075 95
PS02075 96
PS02075 97
PS02075 98
PS02075 99
PS02075 100

```

32	COMMON /FNRGN1/ IOUSE(10),LAST,LAFTER,IGCOMP,IPSO,LT50,IPFL,LTFL,	DE11	2
	*IPFA,LTFA,IPAS,IPASCT,LIXS,LT0XS,LTAXS,IP0S,IEREC,12,14,	FRP0045	1
	216, IFO, IPPC, LTPC, IUELC5, ILENCS, LCMND1, LCMND2,	DE11	4
	JLCMN1, IPASW, LENGP, LLSTEC, IALL, LEVSC, NSC, LENHSM, LENHSM	DE11	5
	*LECDEN, LECENE, LECDIS, IPAF, IPPF	LL9015	4
	*IPPK, LTPK	DS1475	3
	*IBST, IART, IDSS, IBXS, IUPFC, ISFXS, IBFXS, IUFFT, IBFSG, IBFET, IPAXS	DS1475	4
	*IFFC	US1475	5
	*NAME(1), NLC, NDC, LLALCM, ST, LAS	FMH0265	2
32	COMMON/SIMMER/IA(150),FIA(100),A(40710),LASHOR	US1175	1
32	EQUIVALENCE(IA(15),IMF),(IA(16),IMA),(IA(17),IMFS)	PS02075	7A
32	EQUIVALENCE(IA(11),LNUFF),(IA(12),LNGXS),(IA(13),LZ)	FFGEN	14
	*IA(14),LFTEMP),(IA(15),LFSIG),(IA(16),LFFF),(IA(17),LFFXS)	FFGEN	15
	*IA(18),LFSIGO),(IA(19),LFFSS),(IA(20),LFCOM)	FFGEN	1A
	*IA(21),LFCMO),(IA(22),LFNXS),(IA(23),LFDEN)	FFGEN	17
	*IA(24),LFCATMP),(IA(25),IGMT),(IA(26),IMHGM)	FFGEN	1A
	*IA(27),IST),(IA(28),MSIG),(IA(29),MTEM),(IA(30),MCF)	FFGEN	19
32	ITER=1	PS02775	9
33	DO 1 L=1,NC	PS02775	10
34	IF(RHOC(L).LE.1.0E-05) GO TO 1	PS02775	11
37	TEMP(L)=QLOG(TEMP(L))	PD59095	3
50	CONTINUE	PS02775	13
53	DO 3 L=1,NC	PD59115	3
54	IF(RHOC(L).LE.1.0E-05) GO TO 3	PD59115	4
57	I2=COMNXS(L)	PD59115	5
61	NO 2 J=2,I2	PD59115	6
74	NCOM(L,J)=1.0/COMHMO(L,J)	PD59115	7
104	CONTINUE	PD59115	8
107	CALL CLEAN(0.0,SIG0(1),MT)	PD59105	21
120	DO 100 L=1,NC	PS02775	15
121	IF(RHOC(L).LE.1.0E-05) GO TO 100	PS02775	1A
124	I2=COMNXS(L)	PS02775	17
126	DO 100 J=2,I2	PS02775	1A
130	M=COMCOM(L,J)	PS02775	19
134	IF(ITER.EQ.1) GO TO 6	PD59115	9
176	A2N=FXS(3,M,G)+2.0*(C(1MA,M)-FXS(2,M,G)-C(IMFS,M))	PD59115	10
176	FSS1=COMHMO(L,J)*(FSS(1,M,G)+C(IMFS,M)	PD59115	11
	+FSS(2,M,G)+FXS(2,M,G)+SS(4,M,G)+FXS(4,M,G)+X2N)	PD59115	12
221	GO TO 7	PD59115	13
225	FSS1=COMHMO(L,J)+FXS(1,M,G)	PD59115	14
241	CONTINUE	PD59115	15
241	DO 100 L=1,NC	PS02775	21
243	IF(RHOC(L).LE.1.0E-05) GO TO 100	PS02775	22
246	I2=COMNXS(L)	PS02775	23
250	DO 100 JJ=2,I2	PS02775	24
252	MM=COMCOM(L,JJ)	PS02775	25
256	IF(M.EQ.MM) GO TO 100	PD59155	1
260	SIG(MM)=SIGU(MM)+FSS1*NCOM(L,JJ)	PD59115	1A
265	CONTINUE	PS02775	3A
275	CONTINUE	PS02775	37
300	ITER=ITER+1	PS02775	3A
301	DO 500 L=1,NC	FFGEN	21
303	IF(RHOC(L).LE.1.0E-05) GO TO 500	PS90275	21
306	TMIX=TEMP(L)	PS02075	82
306	TMIX2=TMIX*TMIX	PS02075	83
306	I2=COMNXS(L)	FFGEN	23
312	DO 400 J=2,I2	PD59105	22
317	M=COMCOM(L,J)	FFGEN	25
317	NF=NSIGN(M)	PS02075	84
317	N=NF	PS02075	85
317	IFF=1	PD59095	5
324	IF(C(IMF,M).LE.0.0) IFF=2	PD59095	6
333	IF(SIG0(M).LE.1.0E-05) GO TO 170	PD59095	7
336	SIGL=QLOG(SIG0(M))	PD59095	9
345	IF(SIGL.LT.SIG(NF,M)) GO TO 100	PS02075	87
353	DO 80 NN=1,NF	PS02075	8A
355	N=NN	PS02075	89
355	IF(SIGL.GT.SIG(NN,M)) GO TO 100	PS02075	90

365	80	CONTINUE	PS82075	91
367	100	CONTINUE	PUS9095	11
367		IF(N.EQ.1)GO TO 160	PS82075	95
372		IF(N.EQ.NF)GO TO 170	PS82075	96
402		N1 = N-1	FHP9085	9
402		SR=1.0/(SIG(N,M)-SIG(N1,M))	PS82075	97
402		A1=(SIGL-SIG(N1,M))*SR	PS82075	98
411		IF(N.EQ.2)N=3	PS82075	99
417		IF(N.EQ.(NF-1))NF=NF-2	PS82075	100
423		KN=3*(N-1)+1	PS82075	101
423		KN1=KN-3	PS82075	102
423		KL=3*(NF-1)+1	PS82075	103
431		DO 150 K=IFF,4	PS82075	104
460		FN=FCF(KN,K,M)*TMIX2+FCF(KN+1,K,M)*TMIX+FCF(KN+2,K,M)	PS82075	105
460		FT=FCF(1,K,M)*TMIX2+FCF(2,K,M)*TMIX+FCF(3,K,M)	PS82075	106
470		IF(ABS(FN-FT).LE.1.0E-08) GO TO 110	PS82075	107
525		FL=FCF(KL,K,M)*TMIX2+FCF(KL+1,K,M)*TMIX+FCF(KL+2,K,M)	PS82075	108
525		FN1=FCF(KN1,K,M)*TMIX2+FCF(KN1+1,K,M)*TMIX+FCF(KN1+2,K,M)	PS82075	109
534		IF(ABS(FN1-FL).LE.1.0E-08) GO TO 120	PS82075	110
544		IF(FN1.GT.FT)GO TO 120	PUS9095	12
547		IF(FL.GT.FN)GO TO 110	PUS9095	13
552		FB=(FT-FN1)/(FN1-FL)	PS82075	111
552		FA=((FN-FL)/(FT-FN))*FB	PUS9095	14
557		FA=QEXP(A1*QLOG(FA))	PUS9095	16
564		FSS(K,M,G)=(FT*FA+FL*FB)/(FA+FB)	PS82075	113
603		GO TO 150	PS82075	114
607	110	FSS(K,M,G)=FN	PS82075	115
620		GO TO 150	PS82075	116
620	120	FSS(K,M,G)=FN1	PS82075	117
631	150	CONTINUE	PS82075	118
633		GO TO 400	PS82075	119
	C	N=1	PS82075	120
634	160	DO 165 K=IFF,4	PS82075	121
664	165	FSS(K,M,G)=FCF(1,K,M)*TMIX2+FCF(2,K,M)*TMIX+FCF(3,K,M)	PS82075	122
673		GO TO 400	PS82075	123
677	170	KL=3*(NF-1)+1	PS82075	124
702		DO 175 K=IFF,4	PS82075	125
741	175	FSS(K,M,G)=FCF(KL,K,M)*TMIX2+FCF(KL+1,K,M)*TMIX+FCF(KL+2,K,M)	PS82075	126
753	400	CONTINUE	FFGEN	83
756	500	CONTINUE	FFGEN	84
761		IF(ITER.LE.2) GO TO 5	PS82075	22
763		RETURN	FFGEN	85
764		END	FFGEN	86

APPENDIX B

SUBROUTINE CSCAL

CALCULATION OF SHIELDED MICROSCOPIC CROSS SECTION

Following is a listing of subroutine CSCAL which calculates shielded microscopic cross sections. Which isotopes and components to process are specified in the argument of CSCAL. The names and contents of the argument arrays are given below.

Argument Name	Contents
CN(XS,NC)	Number of mix instructions for the j'th component
CN(CM(NC,MTPS)	Mix commands for the j'th component
C(IIN,MT)	Input infinitely dilute microscopic cross section

Argument Name	Contents
CY(IIN,MT)	Output shielded microscopic cross sections
FXS(6,MTPS,IGN)	BRKXS cross-section information (see Table II)
FSS(4,MT,IGN)	Input f-factors
IIN	Number of rows in cross-section table
IGN	Number of energy groups
MT	Total number of problems
NC	Number of components
MTX	MTPS

	SUBROUTINE CSCAL (COMNXX, COMCOM, C, CY, FXS, FSS, IHM, IGM, MT, NC, MTX)	PDS9105	23
23	INTEGER G, COMNXX, COMCOM	CSCAL	3
23	DIMENSION COMNXX(1), COMCOM(NC, 1), C(IHM, MT), FXS(6, MTX, 1)	PS82775	40
	1, FSS(4, MT, IGM)	CSCAL	5
23	DIMENSION CY(IHM, MT)	PDS9105	24
23	COMMON /SIMMER/ IA(150), FIA(100), A(40710), LASWOR	061175	1
23	COMMON /RPASS/ RHOC(10)	CSCAL	7
23	COMMON /FWBGN1/ IDUSE(18), LAST, LASTEC, IGCOMP, IPSO, LT50, IPFL, LTFL,	SE11	2
	*IPFX, LTFX, IPXS, IPXSCT, LIXS, LTOXS, LTAXS, IPQS, IEREC, IC, IA,	FRM9045	1
	216, IFO, IPPC, LTPC, IDELCS, ILENC, LCMRD1, LCMRD2,	SE11	4
	3LCMWR, IPASR, LENG, LLSTEC, IALL, LENSCT, NSC, LENHSM, LENNSM	SE11	5
	*LECDEN, LECENE, LECDIS, IPAF, IPPF	LLS9015	4
	*IPPK, LTPK	051975	3
	*IBST, IBET, IHSS, IBKS, IHFFC, ISFXS, IBFXS, IBFTT, IBFSG, IBFET, IPAXS	051975	4
	*IFFC	051975	5
	*NAME (8), NLC, NQ, LLALCM, STILAS	FRM8265	2
23	COMMON /LOCAL/ ITH, NEHRR, ITH, ISNT, MCR, MTP, MTPS, NISOXS	SE15	7
	1, LMTP, NEXTER, JFISC, IEDIT(2), LIMIT, LENCLR	SE15	3
	*ICONV	051975	6
	*STGLAS	FRM7285	11
23	EQUIVALENCE (IA(80), G) (IA(16), IHA), (IA(9), IHT)	CSCAL	10
23	EQUIVALENCE (IA(10), IHS)	CSCAL	11
23	EQUIVALENCE (IA(11), LNGFF), (IA(112), LNGXS), (IA(113), LZ)	CSCAL	12
	*, (IA(114), LFTMP), (IA(115), LFSIG), (IA(116), LFFF), (IA(117), LFFXS)	CSCAL	13
	*, (IA(118), LFSIG0), (IA(119), LFFSS), (IA(120), LFCOM)	CSCAL	14
	*, (IA(121), LFRHO), (IA(122), LFNXS), (IA(123), LFDEN)	CSCAL	15
	*, (IA(124), LFTMP), (IA(125), IGMT), (IA(126), IHMG)	CSCAL	16
	*, (IA(127), IST), (IA(128), MSIG), (IA(129), MTEM), (IA(130), MCFF)	CSCAL	17
23	EQUIVALENCE (IA(17), IHFS)	PS81875	32
23	DO 400 L=1, NC	CSCAL	20
24	IF (RHOC(L), LE, 1.0E-05) GO TO 400	PS90275	23
27	IT2=COMNXX(L)	CSCAL	23
31	DO 400 J=2, IT2	PDS9105	25
36	M=COMCOM(L, J)	CSCAL	25
36	ABS=C(IHA, M)	PS82775	44
36	SCAT=FXS(3, M, G)	PS82775	45
36	EXTRA=FXS(2, M, G)*C(IHFS, M)-ABS	PS82775	46
36	X2N=SCAT-EXTRA	PS82775	47
36	CY(IHFS, M)=FSS(1, M, G)*C(IHFS, M)	PDS9105	26
36	CY(IHT-1, M)=FSS(1, M, G)*C(IHT-1, M)	PDS9105	27
36	CX=FSS(2, M, G)*FXS(2, M, G)	PS82775	50
36	XX=CX+X2N+CY(IHFS, M)	PDS9105	28
36	CY(IHT, M)=(FSS(3, M, G)*FXS(1, M, G)	PDS9105	29
	1=XX)	PS82775	53
	3*(1.0-FXS(5, M, G))	PS82775	54
	1=XX	PS82775	55
36	ABS=XX-X2N-EXTRA	PS82775	56
36	CY(IHA, M)=ABS	PDS9105	30
36	CY(IHS, M)=CY(IHT, M)-ABS-SCAT+C(IHS, M)-FXS(6, M, G)*FSS(4, M, G)	PDS9105	31
206	IF (G.EQ.1) GO TO 400	PS73075	16
214	CY(IHS+1, M)=FSS(4, M, G-1)*FXS(6, M, G-1)*C(IHS+1, M)	PDS9105	32
	REMAINING DATA REMAINS FIXED	CSCAL	55
	EDIT DATA IF DESIRED	CSCAL	56
243	C 400 CONTINUE	CSCAL	58
251	RETURN	CSCAL	59
252	END	CSCAL	60

APPENDIX C

SUBROUTINE SHLDXS

Following is a listing of subroutine SHLDXS which is the controller for cross section processing — both infinitely dilute and shielded cross sections. The subroutine also calculates the

component microscopic cross sections as well as the macroscopic cross section and then stores macroscopic data on disk. These calculations are performed from line 502 to end of program.

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SUBROUTINE SHLDXS(C,CTOI,DENST,NSIGN,SIGO,IDC
1,FF,COMNXS,COMCOM,CUMRHO,COMDEN,FSS
2,FXS,SF,MIXDEN,MIXNUM,MIXCOM
1,CX
3,IHM,MT,IT,JI,NC,IGM,IGMTT
4)
41  INTEGER COMNXS,COMCOM
41  REAL MIXDEN
41  DIMENSION C(IHM,MT),CTOI(IT,1),DENST(1),NSIGN(1),SIGO(1),IDC(1)
1,FF(1),COMNXS(1),COMCOM(NC,1),CUMRHO(NC,1),COMDEN(NC,1)
2,FSS(4,MT,1),FXS(6),SF(1),MIXDEN(1),MIXNUM(1),MIXCOM(1)
41  DIMENSION CRHO(5),XCND(5),IDK(4)
41  DIMENSION CX(IHM,MT)
41  COMMON/RPASS/RHOC(10)
41  COMMON/STMMER/IA(150),FIA(100),A(40710),LASWOR
41  COMMON /FWBGN1/ IDUSE(18),LAST,LASTEC,IGCOMP,IPSU,LTSO,TPFL,LTFL,
*IPFX,LTFX,IPAS,IPASCT,LIXS,LTOXS,LTAXS,IPQS,IEREC,I4,I4,
2I6,IFU,IPPC,LTPC,IDLCS,ILENCS,LCMR01,LCMR02,
3LCMR01,IPASHW,LENGP,LLSTEC,IALL,LENSCT,NSC,LENNHM,LENNHM
*,LECDEN,LECDENE,LECDIS,IPAF,IPPF
*,IPPK,LTPK
*,IRST,IHET,IBSS,IBXS,IBPFC,ISFXS,IBFXS,IBFTT,IBFSG,IBFET,IPAXS
*,IFFC
*,NAME(R),NLC,NQ,LLALCM,STILAS
41  COMMON/UNITS/NINP,NOUT,NOPS,NAFLUX,NDUMPI,NDUMPO
*,NEXTRA,DMPIN,UMPOUT(2)
*,NFILM,ISNCON,ISOTXS,IBHXS,NFPLT,ICAM
*,UNLAS
41  COMMON /LOCAL/ ITH,NEHUR,ITLIM,ISNT,MCR,MTP,MTPS,NISOXs
1,LMTF,NEXTER,JFISC,IEDIT(2),LIMIT,LENCLE
*,ICONV
*,STSLAS
41  EQUIVALENCE (IA(80),IG),(IA(16),IHA),(IA(10),IHS),(IA(9),IHT)
41  EQUIVALENCE (IA(R),MS)
41  EQUIVALENCE (IA(11),LNGFF),(IA(112),LNGXS),(IA(113),LZ)
*,(IA(114),LFTMP),(IA(115),LFSIG),(IA(116),LFFF),(IA(117),LFFXS)
*,(IA(118),LFSIGO),(IA(119),LFFSS),(IA(120),LFCOM)
*,(IA(121),LFRHO),(IA(122),LFNXS),(IA(123),LFDEN)
*,(IA(124),LFATMP),(IA(125),IGMT),(IA(126),IHMGM)
*,(IA(127),IST),(IA(128),MSIGI),(IA(129),MTEMI),(IA(130),MCFF)
41  CALL SECOND(1)
42  CALL CLEAR(1.0,XCND,5)
45  IF(MTPS,EG,0) GO TO 2
C  HEAD IN SIG VALUES
52  CALL REED(0,IBET,MTPS,SF(1),MTPS*MSIGI,1)
63  CALL REED(0,IBET,NSIGN(1),MTPS,1)
100  MS34=34*MSIGI
100  NLG=MS34*IGM
C  HEAD IN ALL THE BONDARENKO TYPE CROSS SECTION INFORMATION
100  NFLG=6*IGM*MTPS
112  CALL REED(0,IBXS,FXS(1),NFLG,1)
117  CALL CLEAR(1.0,FSS,4*MT*IGM)
133  2  CONTINUE
133  1  IG=1
133  NQPR=2*NC
133  NQK=NQPR*IT
C  REWIND TEMPORARY CROSS SECTION FILE
140  CALL REED (ISOTXS,0,DUM,0,4)
150  5  CONTINUE
150  IF(MTPS,EG,0) GO TO 4
152  ISF=1
C  HEAD IN F-FACTOR TEMPERATURE COEFFICIENTS
152  ISTART=IRST+(IG-1)*MS34
157  DO 3 M=1,MTPS
160  CALL REED(0,ISTART,FF(1SF),MS34,1)
166  ISTART=ISTART+NLG
173  3  ISF=ISF+MS34
200  4  CONTINUE
200  IECD=LECDEN
C  ENTER THE J-TM ROW-DO ALL COLUMNS(IT) FOR ALL IHM TYPES
C  AND NC COMPONENTS

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PS82075 42
SHLDXS 3
SHLDXS 4
PS9105 14
SHLDXS 5
SHLDXS 6
SHLDXS 7
SHLDXS 8
PS82075 43
PS82075 44
SHLDXS 11
SHLDXS 12
PS9105 15
PS81375 1
061175 1
SETI 2
FRP9045 1
SETI 4
SETI 5
LLS9015 4
051975 3
051975 4
051975 5
FRP8265 2
FRP8065 1
FRP8065 2
FRP8185 2
FRP7285 12
SETD 2
SET5 3
051975 6
FRP7285 11
SHLDXS 17
052775 68
SHLDXS 18
SHLDXS 20
SHLDXS 21
SHLDXS 22
SHLDXS 23
SHLDXS 24
SHLDXS 25
PS61875 4
PS82075 45
PS82075 46
PS82075 47
PS82075 49
PS82075 50
PS82075 51
PS82075 52
PS82075 53
PS82075 54
PS9095 1
PS82075 55
SHLDXS 28
SHLDXS 29
SHLDXS 30
SHLDXS 31
SHLDXS 32
SHLDXS 33
PS82075 56
PS82075 57
PS82075 58
PS82075 59
PS82075 62
PS82075 63
PS82075 64
PS82075 65
PS82075 66
PS73075 5
SHLDXS 35
SHLDXS 36

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202		CALL REED(0,IPXS+(IG-1)*LTAS,C,LTXS,1)	PS82075	67
216		IF(MTPS,EQ.0)CALL REED(0,IPXS+(IG-1)*LTXS,CX,LTXS,1)	PS82075	16
227		DO 50 J=1,JT	SHLOXS	37
235		IK=1	SHLOXS	38
	C	READ IN TEMPERATURES AND DENSITIES FROM HYDRODYNAMICS	SHLOXS	39
236		CALL REED (0,IECD,DENST,NRK,1)	SHLOXS	40
241		CALL CLEAR (U,0,CTOT,I)*IHM)	SHLOXS	41
252		DO 30 I=1,IT	SHLOXS	42
257		IF(MTPS,EQ.0) GO TO 1411	PS73075	7
	C	GET TRUE NUMBER DENSITIES	SHLOXS	43
260		DO 6 N=1,NC	PS81375	2
261		MXS=COMNKS(N)	PS81375	3
261		RHO=DENST(IK+N-1)	PS81375	4
261		RHOC(N)=RHO	PS81375	5
270		DO 6 M=1,MXS	PS81375	6
300	6	COMRHO(N,M)=RHO*COMDEN(N,M)	PS81375	7
	C	CALCULATED SIGO VALUES	SHLOXS	40
	C	NOW CALCULATE F-FACTORS FOR GIVEN SIGO AND TEMPERATURE	SHLOXS	56
312		CALL FFGEN(COMNKS,COMCUM,NSIGN,DENST(IK+NC),SF,SIGO, IFF,FSS,C,IG,NC,MSIGI,3*MSIGI,IHM,MT,COMRHO,FXS,M,PSI)	PS82075	68
			PS82075	69
			PS82075	70
350		IF(IG,EQ.1) GO TO 12	PS81875	6
352		ITHM=IT*(J-1)*MT*MT*(I-1)+IBFSG	PS81875	7
362		CALL REED(0,ITHM,SIGO,M!,1)	PS82775	2
366		DO 11 KL=1,MT	PS81875	9
376	11	FSS(4,KL,IG-1)=SIGO(KL)	PS82775	3
414	12	IF(IG,EQ.1GM) GO TO 14	PS81875	11
417		DO 13 KL=1,MT	PS81875	12
423	13	SIGO(KL)=FSS(4,KL,IG)	PS82775	4
433		ITHM=IT*(J-1)*MT*MT*(I-1)+IBFSG	PS81875	14
444		CALL RITE(0,ITHM,SIGO,M!,1)	PS82775	5
457	14	CONTINUE	PS81875	14
	C	CALCULATE SHIELDED CROSS SECTIONS	SHLOXS	62
457		CALL CSCAL(COMNKS,COMCUM,C,CX,FXS,FSS I,IHM,IGM,MT,NC,MTPS)	PS82775	6
475		IF(MCPE,LI.0) GO TO 18	SHLOXS	60
	C	MIX ISOTOPES TO FORM COMPONENTS	SHLOXS	70
502	1411	CONTINUE	PS73075	9
502		IXS=IHT*IG	PS81375	8
504		DO 1000 MM=1,MS	PS81375	9
506		NN=MIXNUM(MM)	PS81375	10
506		LL=MIXCOM(MM)	PS81375	11
506		AD=MIXDEN(MM)	PS81375	12
513		DO 1000 II=1,IXS	PS81375	13
515		IF(LL,EQ.0)GO TO 900	PS81375	14
516		CX(II,NN)=CX(II,NN)+AD*CX(II,LL)	PS82775	18
526		GO TO 1000	PS81375	16
527	900	CX(II,NN)=AD*CX(II,NN)	PS82775	19
536	1000	CONTINUE	PS81375	18
	C	CALCULATE NORMALIZED MACROSCOPIC CROSS SECTION	SHLOXS	73
			SHLOXS	74
543	18	DO 20 N=1,NC	SHLOXS	75
545		M=IDC(N)	SHLOXS	76
545		DENST=DENST(IK+N-1)	SHLOXS	77
551		IF(DENST,EQ.0,0) GO TO 20	SHLOXS	78
553		DO 19 NL=1,IXS	PS81175	7
			SHLOXS	80
566	19	CTOT(I,NL)=CTOT(I,NL)+CA(NL,M)*DENST	PS82775	20
575	20	CONTINUE	SHLOXS	82
600	30	IK=IK+NQPR	SHLOXS	83
604		IECD=TECD+NQK	SHLOXS	84
	C	NOW HAVE ALL IHM CROSS SECTION TYPES FOR ALL I CELLS	SHLOXS	85
	C	FOR FIXED J NOW	SHLOXS	86
605		DO 40 NL=1,IXS	PS81175	8
607		ITHM=IPXSCT+(NL-1)*LTOXS	SHLOXS	88
		I=IT*(J-1)	SHLOXS	89
617	40	CALL RITE (0,ITHM,CTOT(I,NL),IT,1)	SHLOXS	90
634	50	CONTINUE	SHLOXS	91
	C	ALL IT*JT CELLS HAVE BEEN PROCESSED FOR ALL IHM	SHLOXS	92
	C	TYPE CROSS SECTIONS FOR A FIXED ENERGY GROUP. NOW PUT	SHLOXS	93
	C	THIS INFORMATION ONTO DISC.	SHLOXS	94

```

637      DO 60 NL=1,IAS
640      CALL REED(0,IPXSCT,(NL-1)*LTOXS,CTOT,LTOXS,1)
654 60    CALL RITE (ISOTXS,IG,CTOT,LTOXS,2)
666      IG=IG+1
670      IF(IG.LE.IGM)GO TO 5
672      CALL REED(ISOTXS,0,DUM,1,4)
676      CALL SECOND(T2)
324      FORMAT(5H TIME,2E12.5)
704      WRITE(9,324) T2,T1
713      RETURN
714      END

```

```

PS01175    9
SHLUXS     96
SHLUXS     97
SHLUXS     98
SHLUXS     99
SHLUXS    100
SHLUXS    101
SHLUXS    102
SHLUXS    103
SHLUXS    104
PS90275    10

```

APPENDIX D

TIMING STUDY

Following is the output from a typical SIMMER problem. The particular problem was a 4-energy-group problem with a 35 x 37 mesh grid and 11 isotopes. The elapsed time of 12.288 sec in Table D.1 is the time spent calculating the self-shielding factors for 11 isotopes, 4-groups in 1295 mesh cells

and also calculating and storing the macroscopic cross sections. A relative indication of the time spent in each subroutine as well as the time usage in each portion of the subroutine is given in Table D.2.

		0005000	1346700	34	1.54	65.14	0123456789012	I	
		0005100	1347000	49	1.40	66.33	012345678901	I	
		0005200	1347100	94	2.60	69.21	0123456789012345678901	I	
		0005300	1347200	94	2.60	71.89	0123456789012345678901	I	
		0005400	1347300	109	3.10	74.99	01234567890123456789012345	I	
		0005500	1347400	83	2.36	77.36	0123456789012345678	I	
		0005600	1347500	70	1.99	79.35	0123456789012345	I	
		0005700	1347600	60	2.36	81.81	012345678901234567890	I	
		0005800	1350000	22	.63	82.60	012345	I	
		0005900	1350100	32	.91	83.31	01234567	I	
		0006000	1350400	3	.08	83.83	01	I	
		0006100	1350500	4	.11	83.77	01	I	
		0006200	1351300	13	.37	84.19	0123	I	
		0006300	1351400	9	.26	84.44	012	I	
CBCAL	5.70								
		0000250	1355100	6	.17	84.62	01	I	
		0000350	1355200	16	.46	85.08	01234	I	
		0000450	1355300	13	.37	85.45	0123	I	
		0000550	1355400	10	.28	85.73	012	I	
		0000650	1355500	17	.48	86.21	01234	I	
		0000750	1355600	13	.37	86.59	0123	I	
		0001050	1355700	3	.14	86.73	01	I	
		0001150	1356000	11	.31	87.04	012	I	
		0001250	1356100	7	.20	87.24	012	I	
		0001350	1356200	10	.28	87.32	012	I	
		0001450	1356300	11	.31	87.84	012	I	
		0001550	1356400	13	.37	88.21	0123	I	
		0001650	1356500	9	.26	88.46	012	I	
		0001750	1356600	5	.14	88.81	01	I	
		0002050	1356700	10	.28	89.09	012	I	
		0002150	1357000	12	.34	89.23	0123	I	
		0002250	1357100	16	.46	89.69	01234	I	
		0002350	1357200	13	.37	90.06	0123	I	
		0002450	1357300	3	.09	90.13	01	I	
CLEAR	.66								
B3208	4.30	0000130	1360100	22	.63	90.80	012345	I	
		0000510	1360200	121	3.45	94.23	0123456789012345678901234567	I	
		0000110	1360300	30	.85	93.10	01234567	I	
GENP	2.91	7777770	1360400	30	1.42	96.33	012345678901	I	
		0000070	1360500	32	1.40	96.01	012345678901	I	

END OF OVERLAY(02.03)
TOTAL PERCENT IN OVERLAY=97.49