XIX. WIMSR

This module is used to prepare libraries for the reactor-physics code WIMS.[1] WIMS stands for "Winfrith improved multigroup scheme;" it has been developed through its various versions at the UK laboratory AEE/Winfrith. WIMS-E is the current Winfrith version, and it is distributed commercially. WIMS-D is an older version that is freely available through various distribution centers; therefore, it is very popular all around the world.

WIMS uses collision-probability methods for computing fluxes in reactor pin cells and more complicated geometrical arrangements. Therefore, it requires transport, fission, and capture cross sections, a transfer matrix for epithermal neutrons, fission-source information ($\overline{\nu}$ and χ), and a bound-atom scattering matrix for thermal neutrons. Self-shielded cross sections are obtained using equivalence theory from tabulated resonance integrals with intermediate resonance corrections. The resonance integrals can be obtained from the self-shielded cross sections produced by GROUPR, and the intermediate-resonance λ values by group can be computed using the NJOY flux calculator. WIMS libraries normally use a standard 69-group structure with 14 fast groups, 13 resonance groups, and 42 thermal groups.

A. Resonance Integrals

WIMS computes the self-shielded cross sections for a wide range of mixtures and fuel geometries using equivalence theory. The GROUPR chapter of this report describes the narrow-resonance (NR) version of equivalence theory; that is, all systems with the same value for the "sigma-zero,"

$$\sigma_{0i} = \frac{1}{n_i} \left\{ \sum_{j \neq i} n_j \sigma_{tj} + \sigma_e \right\} , \tag{1}$$

in a group have the same self-shielded cross section in that group. Here, n_j is the number density for material j with cross section σ_{tj}, and σ_e is the escape cross section (which takes care of the geometry of the fuel).

However, in the near epithermal range (*e.g.,* 4–100 eV), some resonances are too wide for the NR approximation to apply well. For these resonances, the effect of a moderator material is reduced, because collisions with the moderator do not always result in enough energy loss to remove the neutron from the resonance. For this reason, WIMS uses an intermediate-resonance (IR) extension to equivalence theory in which the background cross section is taken to be the following:

$$\sigma_{Pi} = \frac{1}{n_i} \left\{ \sum_j n_j \lambda_j \sigma_{pj} + \sigma_e \right\} , \tag{2}$$

where the λ factors are numbers between zero and one. Note that σ_p, the potential scattering cross section, is used here, and that the sum is now over all materials. The basic concept is the same: all systems with the same value of the IR "sigma-P" for a group will have the same self-shielded cross sections for that group.

WIMS takes the additional step of expressing the self-shielding data in terms of "resonance integrals," instead of using the self-shielded cross sections produced by GROUPR. That is,

$$\sigma_x(\sigma_0) = \frac{\sigma_P I_x(\sigma_P)}{\sigma_P - I_a(\sigma_P)} , \tag{3}$$

and

$$I_x(\sigma_P) = \frac{\sigma_P \sigma_x(\sigma_0)}{\sigma_P + \sigma_a(\sigma_0)} , \tag{4}$$

where x denotes the reaction, either "a" for absorption or "nf" for nu*fission, and I_x is the corresponding resonance integral.

In order to clarify the meaning of this pair of equations, consider a homogeneous mixture of ^{238}U and hydrogen with concentrations such that there are 50 barns of hydrogen scattering per atom of uranium. The GROUPR flux calculator can be used to solve for the flux in this mixture, and GROUPR can then calculate the corresponding absorption cross section for ^{238}U. Assuming that $\lambda = 0.1$ and $\sigma_p = 10$ for the uranium, the numbers being appropriate for WIMS group 25, we get $\sigma_P = 51$. This value of σ_p goes into the `SIGZ` array in the resonance-integral block on the WIMS library, and the corresponding I_a goes into the `RESA` array.

At some later time, a WIMS user runs a problem for a homogeneous mixture of ^{238}U and hydrogen that matches these specifications. WIMS will compute a value of σ_P of 51.0, interpolate in the table of resonance integrals, and compute a new absorption cross section that is exactly equal to the accurate computed result from the original GROUPR flux-calculator run.

This argument can be extended to more complex systems. For example, the assembly calculated using the flux calculator could represent an enriched uranium-oxide fuel pin of a size typical of a user's reactor system with a water moderator. The computed absorption cross section is converted to a resonance integral and stored with the computed value of σ_P. In any later calculation that happens to mimic the same composition and geometry, WIMS will return the accurate calculated absorption cross section. Equivalence theory, with all its approximations, is only used to interpolate and extrapolate around these calculated values. This is a powerful approach, because it allows a user to optimize the library in order to obtain very accurate results for a limited range of systems without having to modify the methods used in the lattice-physics code. Unfortunately, the present version of WIMSR does not allow you to enter σ_P directly; it computes it from input data that only consider one material at a time. A future version may include the more general capabilities described in this paragraph.

Let us call the homogeneous uranium-hydrogen case discussed above "case 0." Now, consider a homogeneous mixture of ^{238}U, oxygen, and hydrogen. Ratio the number densities to the uranium density such that there is 1 barn/atom of oxygen scattering and 50 barn/atom of hydrogen scattering. Carry out an accurate flux calculation for the mixture, and call the result "case 1." Also do an accurate flux calculation with only hydrogen, but at a density corresponding to 51 barns/atom. Call this result "case 2." The IR lambda value for oxygen is then given by

$$\lambda = \frac{\sigma_a(1) - \sigma_a(0)}{\sigma_a(2) - \sigma_a(0)} \ . \tag{5}$$

Note that λ will be 1 if the oxygen and hydrogen have exactly the same effect on the absorption cross section. In practice, $\lambda = .91$ for WIMS group 27 (which contains the large 6.7 eV resonance of ^{238}U), and $\lambda = 1$ for all the other resonance groups. That is, all the resonances above the 6.7 eV resonance are effectively narrow with respect to oxygen scattering.

Similarly, do a flux-calculator solution for a homogeneous mixture of ^{238}U combined with 1 barn/atom of ^{235}U and 50 barn/atom of hydrogen. Call the result "case 3." Now, the lambda value for ^{235}U is given by

$$\lambda = \frac{\sigma_a(3) - \sigma_a(0)}{\sigma_a(2) - \sigma_a(0)} \ . \tag{6}$$

The actual value obtained for WIMS group 27 is .035. Group 26 gives 0.50, and group 25 gives 0.09. An examination of the flux-calculator equations in the GROUPR chapter of this manual shows that the effect of the "admixed" moderator term depends only on its atomic mass (through the α value); therefore, the IR λ values will be the same for all uranium isotopes (and the same values should work for all the actinides). This conclusion neglects the small effects of absorption in the admixed isotope on the intraresonance flux for one resonance.

Table 1: IR λ Values for Several Resonance Groups and Two Different Reactor Systems

WIMS group	λ(U) U238@50b	λ(O) U238@50b	λ(U) U235@200b	λ(O) U235@200b
27	.035	.91	0.20	1.00
26	.50	1.00	.38	1.00
25	.092	1.00	.44	1.00
24	.090	1.00	.55	1.00
23	.29	1.00	.46	1.00

This process can be continued for additional admixed materials from each important range of atomic mass. The result is the table of λ_{gi} values needed as WIMSR input.

What are the implications of this discussion? Foremost is the observation that the lambda values for the isotopes are a function of the composition of the mixture that was used for the base calculation. To make the effect of this clear, let us consider two different types of cells:

1. a homogeneous mixture of U238 and hydrogen, and
2. a homogeneous mixture of U235 and hydrogen.

A look at the pointwise cross sections in group 27 shows very different pictures for the two uranium isotopes. The U-238 cross section has one large, fairly wide resonance at 6.7 eV, and the U-235 cross section has several narrower resonances scattered across the group. If the lambda values are computed for these two different situations, the results in Table 1 are obtained.

It is clear that the energy dependence of the two lambda sets is quite different. This is because of the difference in the resonance structure between U-238 and U-235. Clearly, the one resonance in group 27 in U-238 is effectively wider than the group of resonances in group 27 for U-235. Group 26 has essentially no resonance character for ^{238}U, which reverses the sense of the difference. In groups 24 and 25, the ^{235}U resonances become more narrow, while the ^{238}U resonances stay fairly wide. Finally, in group 23, the ^{238}U resonances begin to get narrower.

These results imply that completely different sets of lambda values should be used for different fuel/moderator systems, such as U-238/water, U-235/water, or U-238/graphite. In practice, this is rarely done.

The remaining question is, "How should the self-shielded cross sections for the minor isotopes be calculated?" Formally, the best approach using NJOY would be to first do an accurate flux calculation for pure ^{238}U mixed with hydrogen (or to be really accurate, a typical reactor cell containing pure ^{238}U oxide), and to save the resulting flux on a scratch file. This flux would then be used as input for the ^{235}U calculation. (See the GROUPR chapter for details.) This approach takes care of all the complexities of resonance-resonance interference, the drop in the average flux across the group caused by accumulated ^{238}U absorptions, and so on. In practice, this is rarely done. Since the self-shielding effects in the minor actinides are much smaller than those in the main absorber, it is usually sufficient to do a simple NR calculation for the minor actinides and to convert them into WIMS resonance integrals with the normal lambda values for heavy isotopes.

B. Cross Sections

The first part of the WIMS cross section data contains σ_p for the resonance groups (15–27 in the normal 69-group structure), the scattering power per unit lethargy for the resonance groups, the transport cross section for the fast groups (1–27 normally), the absorption cross section for the fast groups, an obsolete quantity for the resonance groups (set to zero), and the intermediate-resonance λ values for the resonance groups. For WIMS-E, the (n,2n) cross section is added between the slowing-down power and the transport cross section.

The σ_p value is assumed to be constant (see `SIGP` in the user input instructions). It must be obtained by finding the scattering length a in the ENDF file and computing $\sigma_p = 4\pi a^2$. The scattering power per unit lethargy is $\xi\sigma_s/\tau$, where ξ is the log energy loss parameter given as MT=252 on the GENDF file, σ_s is the elastic scattering cross section (MT=2), and τ is the lethargy width for the group, which can be calculated from the group structure given in MF=1/MT=451 on the GENDF file. The (n,2n) cross section is obtained from MF=3/MT=16 on the GENDF file. The absorption cross section is computed by adding up the fission cross section (MT=18) and all the cross sections given with MT=102–150. The (n,2n) cross section (MT=16) is then subtracted from the sum. Finally, the λ values are obtained from the user's input. See Section A for more details on these intermediate-resonance corrections.

The next part of the WIMS data file contains the fission neutron production cross section $\overline{\nu}\sigma_f$ and the fission cross section σ_f for the fast groups (1–27 normally). The cross section is always obtained from MT=18 on the GENDF file, but there are several complications involved in getting $\overline{\nu}$.

A shortcut for obtaining the fission data is to run MFD=3/MTD=452 and MFD=5/MTD=452 in GROUPR. This approach ignores the energy dependence of fission neutron emission at high energies and the effects of delayed neutrons on the fission spectrum. If these options are used in GROUPR, it is important not to use the other options described below at the same time. When WIMSR finds a section on the GENDF file with MF=3/MT=452, it can read in $\overline{\nu}\sigma_f$ directly.

A better approach to fission in GROUPR is to prepare a full fission matrix for MT18, or to prepare matrices for all the partial fission reactions, MT=19, 20, 21, and 38. The latter is the recommended approach for evaluations with both MT18 and MT19 given in File 5. See the GROUPR chapter for more details. WIMSR reads in the data given in MF=6/MT=18, or in MF=6/MT19,20,..., and sums over all secondary-energy groups to obtain the prompt part of $\overline{\nu}\sigma_f$. It adds in the delayed part of $\overline{\nu}\sigma_f$ from MF=3/MT=455. If the input GENDF file contains both MT=18 and partial fission matrices, a diagnostic message will be printed, and the partial-fission representation will be used.

The next section of the WIMS data file contains the nonthermal P_0 scattering matrix for incident-energy groups in the fast range (1–27 normally). This matrix is loaded by summing over all of the reactions found on the GENDF tape except the thermal reactions `MTI` and `MTC`. If requested, this matrix is transport corrected by subtracting the sum over secondary-energy groups of the P_1 matrix for each primary group. When the individual reactions are read, they are loaded into "full" matrix (typically 69×69). At the same time, a record is kept of the lowest and highest secondary groups found for each primary group. These limits are then used to pack the scattering matrix into a more compact form.

The scattering matrix is not actively self-shielded in WIMS, but WIMSR allows the user to request that the elastic component be evaluated at some reference σ_0 value different from infinity. This option can be useful for the major fertile component of reactor fuel, that is, for ^{238}U in pins of a uranium system, or for ^{232}Th for fuel in a Thorium/U233 system.

Because the thermal scattering matrix depends on temperature, the next component of the WIMSR data contains the `NTEMP` versions of the basic cross sections and the P_0 scattering matrix for the thermal groups (28–69 normally). The cross sections included are transport, absorption, nu*fission, and fission. The transport positions contain the sum of the thermal inelastic cross section obtained by summing up the P_0 matrix (MF=6/MT=MTI), the thermal elastic cross section from the diagonal elements of the P_0 matrix (MF=6/MT=MTC), if present, and the absorption cross section. If separate P_1 matrices are not given for this material, the

P_1 cross section obtained by summing the P_1 matrices over secondary groups for each primary group is subtracted. The matrix data are read from sections on the GENDF file with MF=6/MT=MTI and MF=6/MT=MTC (if present). As for the temperature-independent matrices, they can be transport-corrected by subtracting the sum over secondary groups of the P_1 matrix for each primary group from the self-scatter position. Also, minimum and maximum limits on the secondary group are determined for each primary group, and the matrix is compacted for efficiency.

The next part of the WIMS data file contains the resonance data, which were discussed in Section XIX.A.

In some cases, these resonance data are followed by a fission spectrum block. The complications of obtaining the fission spectrum are the same as those described above for obtaining the fission neutron production cross section, $\overline{\nu}\sigma_f$. If the shortcut option was used in GROUPR, the fission spectrum can be read directly from MF=5/MT=452 on the GENDF file. The sum over groups is also accumulated in `CNORM` in order to allow the final spectrum to be normalized accurately. The shortcut approach neglects the effects of delayed neutron emission on the fission spectrum.

If fission matrices are available (either MT18, or MT19+20+21...), the prompt part of the fission spectrum is obtained by summing $\sigma_{gg'}\phi_g$ over all primary groups, g. These numbers are also summed into `CNORM` for use later in normalizing χ. The delayed part is obtained as

$$\left\{\sum_g \nu_d \sigma_{fg} \phi_g\right\} \chi_{dg'} \;, \tag{7}$$

which also contributes to the normalization. Note that the energy dependence of the fission matrix is factored into the final χ in proportion to the weighting flux used in GROUPR to prepare the WIMSR input file. For thermal reactor problems, it is easy to provide a good estimate for this weighting flux.

The final block on the WIMS data tape is optional. If present, it contains P_1 scattering matrices for each temperature. These matrices are defined over the entire group range (normally 1–69), and they contain both the temperature-independent and temperature-dependent reactions in each matrix. The methods used to build up these matrices are parallel to those discussed above for the P_0 matrices. Note that if P_1 matrices are given, the transport corrections are not included in the transport cross sections or P_0 matrices.

C. Burn Data

WIMS uses a simplified burn model for tracking the production and depletion of actinides and fission products, and the chains used are hard-wired into the code. WIMSR provides a method to enter new fission-yield data into the WIMS library format, but it has not been used or tested very much so far.

D. User Input

The following user input specifications were copied from the comment cards at the beginning of the WIMSR source. It is always a good idea to check the comment cards in the current version to see if there have been any changes.

```
C     *---INPUT SPECIFICATIONS (FREE FORMAT)---------------------------*
C     *                                                                *
C     * CARD 1                                                         *
C     *    NGENDF  UNIT FOR INPUT GENDF TAPE                           *
C     *    NOUT    UNIT FOR OUTPUT WIMS TAPE                           *
C     *                                                                *
C     * CARD 2                                                         *
C     *    IPRINT  PRINT OPTION                                        *
C     *               0=MINIMUM (DEFAULT)                              *
C     *               1=REGULAR                                        *
C     *               2=1+INTERMEDIATE RESULTS                         *
C     *    IVERW   WIMS VERSION                                        *
C     *               4=WIMS-D (DEFAULT)                               *
C     *               5=WIMS-E                                         *
C     *    IGROUP  GROUP OPTION                                        *
C     *               0=69 GROUPS (DEFAULT)                            *
C     *               9=USER'S CHOICE                                  *
C     *                                                                *
C     * CARD 2A  (IGROUP.EQ.9 ONLY)                                    *
C     *    NGND    NUMBER OF GROUPS                                    *
C     *    NFG     NUMBER OF FAST GROUPS                               *
C     *    NRG     NUMBER OF RESONANCE GROUPS                          *
C     *    IGREF   REFERENCE GROUP (DEFAULT IS LAST FAST GROUP)        *
C     *                                                                *
C     * CARD 3                                                         *
C     *    MAT     ENDF MAT NUMBER OF THE MATERIAL TO BE PROCESSED     *
C     *    NFID    IDENTIFICATION OF MATERIAL FOR THE WIMS LIBRARY     *
C     *    RDFID   IDENTIFICATION NUMBER FOR THE RESONANCE DATA        *
C     *    IBURN   BURNUP DATA OPTION                                  *
C     *               0=NO BURNUP DATA IS PROVIDED (DEFAULT)           *
C     *               1=BURNUP DATA IS PROVIDED IN CARDS 5 AND 6       *
C     *                                                                *
C     * CARD  4                                                        *
C     *    NTEMP   NO. OF TEMPERATURES TO PROCESS FOR THIS MATERIAL    *
C     *               (0=ALL FOUND ON INPUT TAPE)                      *
C     *    NSIGZ   NO. OF SIGMA ZEROES TO PROCESS FOR THIS MATERIAL    *
C     *               (0=ALL FOUND ON INPUT TAPE)                      *
```

```
C     *    SGREF   REFERENCE SIGMA ZERO                                *
C     *    IRES    RESONANCE ABSORBER INDICATOR (0=NO,1=YES)           *
C     *    SIGP    POTENTIAL CROSS SECTION FROM ENDF/B.                *
C     *    MTI     THERMAL INELASTIC MT (DEFAULT=0=NONE)               *
C     *    MTC     THERMAL ELASTIC MT (DEFAULT=0=NONE)                 *
C     *    IP1OPT  INCLUDE P1 MATRICES                                 *
C     *               0=YES                                            *
C     *               1=NO, CORRECT P0 INGROUPS (DEFAULT)              *
C     *    INORF   RESONANCE FISSION (IF FOUND)                        *
C     *               0=INCLUDE RESONANCE FISSION (DEFAULT)            *
C     *               1=DO NOT INCLUDE                                 *
C     *    ISOF    FISSION SPECTRUM                                    *
C     *               0=DO NOT INCLUDE FISSION SPECTRUM (DEFAULT)      *
C     *               1=INCLUDE FISSION SPECTRUM                       *
C     *    IFPROD  FISSION PRODUCT FLAG                                *
C     *               0=NOT A FISSION PRODUCT (DEFAULT)                *
C     *               1=FISSION PRODUCT, NO RESONANCE TABLES           *
C     *               2=FISSION PRODUCT, RESONANCE TABLES              *
C     *                                                                *
C     *   FOLLOWING TWO CARDS ARE FOR IBURN GT 0 ONLY                  *
C     * CARD  5                                                        *
C     *    NTIS    NO. OF TIME-DEPENDENT ISOTOPES                      *
C     *    EFISS   ENERGY RELEASED PER FISSION                         *
C     *                                                                *
C     * CARD  6  (REPEAT THIS CARD NTIS TIMES)                         *
C     *    IDENTA  IDENT OF FISSION PRODUCT ISOTOPE                    *
C     *    YIELD   FISSION YIELD OF IDENTA FROM BURNUP OF MAT          *
C     *                                                                *
C     * CARD  7                                                        *
C     *    LAMBDA  RESONANCE-GROUP GOLDSTEIN LAMBDAS (13 FOR           *
C     *            DEFAULT 69-GROUP STRUCTURE, NRG OTHERWISE).         *
C     *                                                                *
C     ******************************************************************
```

The first card specifies the input and output unit numbers, as is normal for NJOY modules. `NGENDF` comes from a previous GROUPR run, and it can be in either binary or ASCII mode. `NOUT` is always in ASCII mode.

The options card allows the user to select how much detail will be printed on the output listing (`IPRINT`), whether the output is intended for WIMS-D or WIMS-E (`IVERW`), and how many groups are desired. Currently, the only difference between WIMS-D and WIMS-E output is that some additional reaction cross sections are included for the latter. If the user selects some group structure different from the standard 69-group structure, an additional input card is required to give the number of groups (`NGND`), the number of fast groups (`NFG`, 14 for 69 groups), the number of resonance groups (`NRG`, 13 for 69 groups), and the reference group used for normalizing the flux (`IGREF`, normally the low-energy group of the fast groups).

Card three is always required. It gives the ENDF MAT number for the materials to be processed. If this MAT doesn't appear on the GENDF tape, a fatal error message will be issued. `NFID` will be the identification number for this material used on the output WIMS library, and `RDFID` will be the identification number for the resonance data. Formally, WIMS libraries allow for data sets with more than one version of the resonance-integral tabulation. The last parameter on this card is `IBURN` to flag whether burn data are included in the input stream.

The next card starts out with `NTEMP` and `NSIGZ`, which define the size of the resonance-integral tables. They are normally both set to zero; the code then uses all of the values computed by GROUPR. The reference sigma-zero value, `SGREF`, is used for the elastic cross section and matrix, because these quantities are not normally self-shielded by WIMS. Normally, `1E10` is appropriate, but for the major fissionable material in the reactor (*i.e.,* U-238 or Th-232), it may be better to use a realistic number like `SGREF=50`. WIMSR assumes that the potential scattering cross section for the material is constant, but this constant value is not available from the GROUPR output. The WIMSR user will have to look in the ENDF-format evaluation for the scattering length a, compute $\sigma_p = 4\pi a^2$, and enter the value as `SIGP`. The following fragment shows where to find the scattering length (`9.56630- 1` in this case):

```
...
9.22350+ 4 2.33025+ 2          0          0          1          01395 2151
9.22350+ 4 1.00000+ 0          0          1          2          01395 2151
1.00000+ 0 8.20000+ 1          1          1          0          01395 2151
3.50000+ 0 9.56630- 1          0          0          1          01395 2151
2.33025+ 2 0.00000+ 0          0          0        780        1301395 2151
...
```

The parameters `MTI` and `MTC` select the thermal inelastic and elastic data from the sections that might be available on the GENDF tape. Most materials have only free-gas scattering available, and the appropriate values would be `MTI=221` and `MTC=0`. The conventional values to use for reactor moderator materials are given in Table 2.

WIMSR allows P_1 scattering to be treated in two ways. If `IP1OPT=1`, the P_1 matrix for the material is written to the WIMS output file explicitely. This option is normally used only for major moderator materials, such as the components of water. The other option, `IP1OPT=1`, instructs the code to use the P_1 data to transport-correct the P_0 elastic scattering matrix; that is, the ingroup elements of the P_0 matrix are reduced by the sum over all outgoing groups of the P_1 matrix for that ingoing group.

Table 2: Conventional Values for the Thermal MT Numbers (MTI and MTE) Used in WIMSR, GROUPR, and THERMR

Thermal Material	MTI Value	MTC Value
H in H_2O	222	
D in D_2O	228	
Be metal	231	232
Graphite	229	230
Methane	227	
Zr in ZrH	235	236
H in ZrH	225	226
BeO	233	234
H in Polyethylene	223	224

The INORF parameter can be set to 1 to eliminate the resonance-integral table for nu*fission from the WIMS output. Some of the higher actinides are treated this way for some WIMS libraries. The ISOF flag is set to 1 to tell WIMSR to produce a fission spectrum. This is usually done for main fissile materials, such as ^{235}U and ^{239}Pu. The IFPROD flag is used to control whether resonance tables are included for fission products.

WIMSR has some capability to format burn data for incorporation into a WIMS library (see cards 5 and 6). This part of the code has not been used or tested very much.

The final card gives the intermediate-resonance λ values for each of the resonance groups. Methods for obtaining these quantities with NJOY are outlined in Section XIX.A.

E. Coding Details

WIMSR starts by allocating dynamic storage for NAMAX=100000 words. Note that the first 7500 words of this area are reserved for a scratch area called SCR. In some cases, error messages may appear that suggest that this number be increased. The scratch files needed by WIMSR use the unit numbers from 10 through 14.

The next step is to read and echo the user's input. Subroutine WMINIT is then called. It looks at the record MF=1/MT=451 for the desired material on the input GENDF tape to obtain the group structure. It then reads through the entire GENDF tape for this material to set the fission flags I318 and I618 and to count the number of temperatures that are available. The fission flag is used to handle cases where both MT18 and the partial fission representation (MT19, 20, ...) appear on the GENDF tape.

Subroutine `RESINT` is called next to compute the WIMS resonance integrals from the GROUPR self-shielded cross sections. It reads through the entire GENDF tape and extracts the flux, absorption cross section, fission cross section, and elastic cross section versus temperature and sigma-zero for all of the resonance groups. It also extracts the reference-group flux versus temperature and sigma-zero and the fission $\overline{\nu}$ value. The latter is computed from File 6 with delayed contributions from MT=455 in File 3. Once all the data are in place, `RESINT` uses the $\overline{\nu}$ values to convert the self-shielded fission cross sections into self-shielded $\overline{\nu}\sigma_f$ values.

If the user has asked for a value of `NTEMP` that is larger than the number of temperatures on the GENDF tape for this material, `RESINT` will duplicate the values from the last temperature given into the higher temperature positions for the flux and the absorption cross section.

The final step in `WMINIT` is to convert the self-shielded cross sections into resonance integrals using the method described in Section XIX.A. These resonance integrals are written out to a scratch file and displayed on the output listing using subroutine `RSIOUT`. The elastic resonance integrals are only written for WIMS-E.

Next, the main program calls `XSECS` to process the cross sections. The outermost loop is over temperature. A distinction has to be made between the temperature-independent matrix data, such as (n,2n) and (n,n′) reactions, and the temperature-dependent matrix data, such as thermal scattering. While reading through the GENDF tape, the following quantities are extracted and stored using the pointer indicated:

`IABS1`	radiative capture (MT102);
`IABS2`	other absorption reactions (MT=103–150);
`LOCSF0`	the fission cross section (MT18);
`LOCAB0`	also the fission cross section (MT18);
`IN2N`	the (n,2n) cross section;
`ISCAT`	the elastic scattering cross section (MT2), possibly using the value corresponding to the reference sigma-zero value instead of infinite dilution;
`IXI`	the log slowing down ξ (MT252);
`LOCNUS`	the fission yield $\overline{\nu}\sigma_f$ computed from either 3/452 or File 6 plus the delayed part from 3/455;

`LOCCHI`	the fission spectrum χ computed from either 5/455 or File 6 plus the delayed contributions from MT455;
`XS`	the temperature-dependent scattering matrix, containing `MTI` and `MTC`, the thermal inelastic and elastic reactions, respectively;
`L1`	the smallest group number for a nonzero element of the nonelastic part of the matrix stored in `XS`;
`L1E`	the smallest group number for a nonzero element of the elastic part of the matrix stored in `XS`;
`L2`	the largest group number for a nonzero element of the nonelastic part of the matrix stored in `XS`;
`L2E`	the largest group number for a nonzero element of the elastic part of the matrix stored in `XS`; and
`CSIGP1`	the P_1 cross section for the thermal matrix obtained by summing over the P_1 matrix elements for scattering from each group.

Once all the data for a temperature have been stored in memory, several additional operations are performed on them. The initial absorption cross section located at `LOCABO` contains the fission cross section. The final value is formed by adding the data at `IABS1` and `IABS2`, and then subtracting the (n,2n) cross section at `IN2N`. The final transport cross section located at `LOCXTR` is formed by adding the absorption and subtracting the transport correction (`CSIGP1`). The slowing-down power per unit lethargy is computed from ξ at `IXI`, σ_{scat} at `ISCAT`, and the group boundary energies at `IEGB`.

As usual, the treatment of fission is more complex. For some combinations of options, $\overline{\nu}$ is computed by dividing the fission neutron production cross section by the fission cross section, and for others, the value of $\overline{\nu}\sigma_f$ has to be computed from $\overline{\nu}$ and σ_f. In addition, the fission spectrum, if requested, is normalized.

Subroutine `XSECO` starts with a section that writes and prints the temperature-independent part of the WIMS data. This section is skipped when `XSECO` is called with `ITEMP>1`. It first processes the temperature-independent vectors: potential scattering, slowing-down power, transport, absorption, IR lambda, and sometimes (n,2n). Next, it processes the fission vectors nu*sigf and sigf. The temperature-independent part of the scattering matrix includes the fast groups and the resonance groups (this normally totals 27 groups). It is packed by retrieving the low (`LONE`) and high (`LTWO`) limits for each band of nonzero elements from `L1` and `L2`, which were loaded in `XSECS`. They are used to compute the number of elements in the band and the location of the self-scatter element in the band (always 1 for this part of the matrix, because there is no upscatter). They are also used to direct how the numbers in XS are moved into ISCR with the zeros outside of the band removed. Note that the data are stored as follows: location of self-scatter for group 1, number of elements in band for group1, the band of elements for group 1, location of self-scatter for group 2, number of elements in group 2, the band of elements for group 2, etc. If the number of elements in a band is zero, the two counts are there, but no band data are given. After being printed, the temperature-independent part of the matrix is written out on a scratch file NSCR2.

The next part of XSECO is executed for ITEMP=1 and all the higher temperatures. It prints and writes the temperature-dependent transport, and absorption cross sections (they are defined in the thermal range only, normally groups 28–69). Note that the absorption cross section is also written out on scratch file NSCR3. If available, the temperature-dependent fission neutron production cross section and fission cross section are also printed and written. The temperature-dependent scattering matrix is processed as described above, except that the incident-neutron group range is limited to the thermal range (normally 28–69). Note that the location of the self-scatter element will no longer be 1 for these data, because of the presence of upscatter. The packed matrix length and the packed data are written out to scratch file NSCR3.

If the user has requested that P_1 scattering matrices be constructed for the material, subroutine P1SCAT is called. It uses methods similar to those described above. The results are printed and written onto NSCR4 by P1SOUT.

The last step in WIMSR is to call WIMOUT to prepare the final WIMS data library. The first card on NOUT is slightly different for WIMS-D and WIMS-E. It is followed by lines for the burnup data using numbers obtained from common storage.

The data needed for the material identifier card are available in common storage. The temperature-independent data are read from NSCR2 and written to NOUT. Similarly, the temperature-dependent data are read from NSCR3 (although the TEMPR array is obtained from common storage). For WIMS-D, a record mark is written at this point.

The resonance data, if needed, are read from NSCR1 and written to NOUT. The format is slightly different for WIMS-D and WIMS-E. The WIMS-D version has extra lines containing NTNP, the product of the number of temperatures and the number of sigma-zero values, and it has a record mark after the resonance data block. The WIMS-E version has an extra section of resonance-integral data for computing the self-shielded elastic scattering cross section.

If a fission spectrum was requested, it is written out next by using data from the dynamic storage pointer IUFF. If a P_1 matrix was requested, it is read in from NSCR4 and written out onto NOUT.

This completes the entire WIMS library. The final step takes place in the main WIMSR program, where the normal timing and storage usage messages are printed.

F. WIMS Data File Format

The following section describes the WIMS data output provided by WIMSR. It consists of a number of logical blocks of information written out in coded form. The output is intended to be used by a library maintenance code to prepare a binary library for use by the WIMS code.

Library Header (2I5)

NFID	material identifier
NPOS	position to insert material on a large multimaterial library (given for WIMS-E only)

Burnup Data (3(1PE15.8,I6))

(YIELD(I),IFISP(I),I=1,JCC/2 fission yields and fission product flag

Material Identifier Data (I6,1PE15.8,5I6)

IDENT	material identifier
AWR	atomic weight ratio to neutron
IZNUM	atomic charge number Z for this material
IFIS	fission and resonance flag: 0=non-fissile with no resonance tabulation, 1=non-fissile with resonance absorption only, 2=fissile with resonance absorption only (*e.g.,* Pu-240), 3=fissile with resonance absorption and fission, 4=fissile with no resonance tabulations.
NTEMP	number of temperatures
NRESTB	number of resonance tables included (0 or 1)
ISOF	fission spectrum flag (0=no, 1=yes)

Temperature-Independent Vectors (1P5E15.8)

(SIGP(I),I=1,N2)	σ_p for resonance groups
(XX(I),I=1,N2)	$\xi\sigma_s/\tau$ for resonance groups
(XTR(I),I=1,N1+N2)	transport cross section for fast and resonance groups
(ABS(I),I=N1+N2)	absorption cross section for fast and resonance groups
(DUM,I=1,N2)	unused dummy for resonance groups
(ALAM(I),I=1,N2)	IR λ values for resonance groups

Temperature-Independent Fission (IFIS>1 only) (1P5E15.8)

(NSIGF(I),I=1,N1)	$\overline{\nu}\sigma_f$ for fast and resonance groups
(SIGF(I),I=1,N1)	σ_f for fast and resonance groups

P_0 Matrix Length (I15)

NDAT	length of P_0 scattering block to follow

Temperature-Independent P_0 Matrix (1PE15.8)

(XS(I),I=1,NDAT)	packed scattering data: IS for group 1, NS for group 1, NS scattering elements for group 1, IS for group 2, NS for group 2, etc., through all of the fast and resonance groups (normally through group 27). IS is the position of self-scatter in the band of scattering elements (always 1 here), and NS is the number of elements in the band.

Temperature Values (1PE15.8)

(TEMP(I),I=1,NTEMP)	temperatures in Kelvin

Repeat the following 4 blocks for each of the NTEMP *temperatures.*

Temperature-Dependent Transport and Absorption (1PE15.8)

(XTR(I),I=1,N3)	transport cross section for thermal groups
(ABS(I),I=1,N3)	absorption cross section for thermal groups

Temperature-Dependent Fission Vectors (1PE15.8)

(NSIGF(I),I=1,N3)	fission neutron production cross section $\overline{\nu}\sigma_f$ for thermal groups
(SIGF(I),I=1,N3)	fission cross section σ_f for thermal groups

Temperature-Dependent P_0 Matrix Length (I15)

NDAT	length of P_0 scattering block

Temperature-Dependent P_0 Matrix (1PE15.8)

XS(I),I=1,NDAT)	packed scattering data: IS for group N, NS for group N, NS scattering elements for group N, IS for group N+1, NS for group N+1, etc., through the last group (normally group 69). IS is the position of self-scatter in the band of scattering elements, and NS is the number of elements in the band.

Record Mark (' 999999999999'), WIMS-D only

Resonance Control Data

RID	resonance set identifier
NTEMP	number of temperatures for this resonance set
NSIGZ	number of background cross section values

Absorption Resonance Data

(TEMP(I),I=1,NTEMP)	temperatures
(SIGZ(I),I=1,NSIGZ)	background cross section values
(RESA(I),I=1,NTEMP*NSIGZ	absorption resonance integrals

Nu*fission Resonance Data

(TEMP(I),I=1,NTEMP)	temperatures
(SIGZ(I),I=1,NSIGZ)	background cross section values
(RESNF(I),I=1,NTEMP*NSIGZ	nu*fission resonance integrals

Scattering Resonance Data, WIMS-E only

(TEMP(I),I=1,NTEMP)	temperatures
(SIGZ(I),I=1,NSIGZ)	background cross section values
(RESS(I),I=1,NTEMP*NSIGZ	scattering resonance integrals

Record Mark (' 999999999999'), WIMS-D only

Fission Spectrum

(FSPECT(I),I=1,NGND)	fission spectrum χ

Repeat the following two blocks
for each of NTEMP *temperatures.*

P_1 Matrix Length (I15)

NDAT	length of P_1 scattering block

P_1 Matrix (1PE15.8)

XS(I),I=1,NDAT)	packed scattering data: IS for group 1, NS for group 1, NS scattering elements for group 1, IS for group 2, NS for group 2, etc., through the last group (normally group 69). IS is the position of self-scatter in the band of scattering elements, and NS is the number of elements in the band.

G. WIMSR Auxiliary Codes

The WIMSR output as described above is not directly usable by WIMS. Two library-maintenance codes are used at Los Alamos. FIXER is used to modify (fix up) an existing WIMS-D library, or to create a new one, using WIMSR output. It processes burnup data, main data, resonance data, and P_1 matrices. In its fix-up mode, it can replace, delete, or add a material. WRITER is a code to read a WIMS-D library in coded form, convert it to binary form, and list it in a user readable form.

H. Error Messages

ERROR IN WMINIT***DESIRED MATERIAL IS NOT ON GENDF TAPE

Check whether the right input GENDF input tape was mounted.

`ERROR IN WMINIT***INCORRECT GROUP STRUCTURE`

The group structure on the input GENDF file does not agree with the one specified in the WIMSR input deck.

`MESSAGE FROM WMINIT***MAT xxxx MF xx HAS BOTH MT18 AND ...`

If both MT18 and MT19 are present in File 3 or File 6, WIMSR must make a choice of which to use. For materials with partial fission reactions, GROUPR normally does not process the fission matrix from MT18. It is more accurate to use the sum of the partial fission matrices.

`ERROR IN RESINT***STORAGE EXCEEDED`

It will be necessary to increase `NWSCR`, which is currently set to 7500 by a statement in the WIMSR routine.

`ERROR IN XSECS***STORAGE EXCEEDED`

It will be necessary to increase `NWSCR`, which is currently set to 7500 by a statement in the WIMSR routine.

`MESSAGE FROM XSECS***USE ONLY xx TEMPS FOR MAT xxxx`

The thermal inelastic sections are missing from some of the higher temperatures on the input GENDF tape. This message tells you how many temperatures can be used correctly. Check the THERMR and GROUPR runs if more temperatures are needed.

`ERROR IN XSECO***SCRATCH STORAGE EXCEEDED`

It will be necessary to increase `NWSCR`, which is currently set to 7500 by a statement in the WIMSR routine.

`ERROR IN P1SCAT***STORAGE EXCEEDED`

It will be necessary to increase `NWSCR`, which is currently set to 7500 by a statement in the WIMSR routine.

`ERROR IN P1SCAT***NO P1 MATRICES FOUND FOR MAT xxxx`

Check the GROUPR run to make sure that P_1 matrices have been requested for the desired materials.

`ERROR IN P1SCAT***NO TEMPERATURE-DEPENDENT REACTIONS ...`

Check the GROUPR run to make sure that the elastic scattering matrix was requested.

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J. References

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