Upgrades to the WIMS-ANL Code*

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Presented at the 1998 International Meeting
on Reduced Enrichment for Research and Test Reactors

October 18-23, 1998
Sao Paulo, Brazil

*Work supported by the U. S. Department of Energy
Office of Nonproliferation and National Security
under Contract No. W-31-109-ENG-38.

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ABSTRACT

The dusty old source code in WIMS-D4M has been completely rewritten to conform more closely with current FORTRAN coding practices. The revised code contains many improvements in appearance, error checking and in control of the output. The output is now tabulated to fit the typical 80 column window or terminal screen. The Segev method for resonance integral interpolation is now an option. Most of the dimension limitations have been removed and replaced with variable dimensions within a compile-time fixed container. The library is no longer restricted to the 69 energy group structure, and two new libraries have been generated for use with the code. The new libraries are both based on ENDF/B-VI data with one having the original 69 energy group structure and the second with a 172 group structure. The common source code can be used with PCs using both Windows 95 and NT, with a Linux based operating system and with UNIX based workstations. Comparisons of this version of the code to earlier evaluations with ENDF/B-V are provided, as well as, comparisons with the new libraries.

Introduction

The present WIMS-ANL code has evolved from the original UNIX version of the WIMS-D4 code and library.[1-4] The first set of modifications included the ability to generate both macroscopic and microscopic multi-group cross sections in the standard ISOTXS format with burnup dependent data. The modifications also included the capability to selectively represent up to 35 separate fission product isotopes plus a lumped fission product. This early version of the code was designated WIMS-D4m.

The original 69 energy group library was completely replaced by ENDF/B-V based data. The library was enhanced to include a secondary file that provides more detailed data. In the secondary file the capture and scattering data are broken down into their components (n,alpha; n,p; n,2n; etc.) along with full P1 scattering data for each isotope. The ability to still use the original library and/or a single file with the new library has been maintained. This required extensive upgrades to the WIMSR module

in the NJOY code[5] in order to write the proper library file(s). The library files are typically generated in an ASCII format for portability and converted to binary with an auxiliary editor/converter code.

The next modification was the addition of the Supercell option.[4] This option eliminates some of the limitations inherent in the standard options. The Supercell option is well suited to the treatment of complex geometries, experiment, reflector and control regions, and the treatment of multiple resonance materials in the same model. This version of the code was given the label WIMS-D4M (an upper case M to indicate a more major modification to the WIMS-D4 version of the code). This version of the code also included a capability for generating separate and lumped fission product data for use with the MCNP code.[6]

The latest version of the WIMS code, WIMS-ANL, includes a major revision in the FORTRAN source code. The capabilities of this version of the code are summarized, results from this version are compared with earlier results and new libraries for the code are described in the following sections.

The WIMS-ANL Code

The WIMS-ANL version of the code has FORTRAN source code that is almost entirely variably dimensioned and reflects more modern programming practices. The source code is cleaned up with all unused sections of code and keywords removed. All of the common blocks and fixed parameters have been relocated to two INCLUDE files. Modifications to fixed parameters and default settings can easily be made. The revised source code is completely FORTRAN 77 compatible, but the same source code has also been compiled successfully with a FORTRAN 90 compiler. The code runs interactively on PCs with Windows 95 and Windows NT, and can also be compiled and run with the Linux operating system. WIMS-ANL has one common set of source code for all of the operating systems. The PC configured source code can be converted to either UNIX or Linux by using a companion preprocessor code. The preprocessor code also generates the appropriate MAKEFILE for compiling the code on the corresponding system.

The output from the code has been completely rewritten to conform with viewing the results on a 80 column PC, workstation or terminal screen. The output is displayed in tabular form where possible making the output very readable. An example of the output is provided in Figure 1. The output content now is completely under the user's control, and the default edits can be customized to the desires of the user group. In Fig. 1 microscopic cross section data are being saved for Sm-149 (as S490), and for the default edits only the principal cross section data would be listed in the edits, i.e. Transport, Total, Capture, [(N,Alpha), (N,P) and (N,2N) only present if a secondary library file is included] data. The Total Production Matrix data is listed here only because the user specifically requested these data in the input. This is only a partial listing of the data for S490. Since a secondary library file was provided the edits of the scattering data would also include scattering matrices for the elastic, inelastic and n,2n components. These edits would follow those shown in the figure. Output edits that would normally be in the default set of edits can likewise be eliminated at the user's request. The user may elect to turn on all available edits regardless of the default settings. With all of the edits turned on the output control keywords in the original code may be used as before, but the new scheme of output control is far superior to use.

The error checking and error messages generated have been significantly upgraded in this version of the code. The cross sections library files are checked for consistency. The messages generated are generally quite informative and useful. There are no longer just terse messages such as "STOP 1000".

```
DATA FOR NUCLIDE  S490 1  :

       Basic data source:     WIMS4M
           Material I.D.:     ENDF/B
             Atomic mass:  1.48917E+02
      Energy per fission:  0.00000E+00
      Energy per capture:  1.27846E-12
             Temperature:  3.00000E+02
    Potential scatt xsec:  3.25950E+00
            Atom density:  2.56111E-19
                   Class:    Undefined


   Cross-Sections:
   --------------

   Broad Grp    Transport        Total      Capture
           1  4.14189E+00  6.88164E+00  8.09330E-02
           2  1.23037E+01* 1.08743E+01  1.51364E+00
           3  1.90321E+02  1.93102E+02  1.25806E+02
           4  1.22125E+03  1.22217E+03  1.20535E+03
           5  1.18048E+03  1.18078E+03  1.15747E+03
           6  7.17483E+04  7.17556E+04  7.11691E+04
           7  4.43507E+04  4.43509E+04  4.41704E+04

   Broad Grp      N,Alpha          N,P         N,2N
           1  1.77796E-04  1.77796E-04  1.46792E-02
           2  0.00000E+00  0.00000E+00  0.00000E+00
           3  0.00000E+00  0.00000E+00  0.00000E+00
           4  0.00000E+00  0.00000E+00  0.00000E+00
           5  0.00000E+00  0.00000E+00  0.00000E+00
           6  0.00000E+00  0.00000E+00  0.00000E+00
           7  0.00000E+00  0.00000E+00  0.00000E+00


   Total Production Matrix:
   ------------------------

   P0 To Grp  From Grp  1  From Grp  2  From Grp  3  From Grp  4  From Grp  5
           1  5.69957E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
           2  1.11539E+00  9.33183E+00  0.00000E+00  0.00000E+00  0.00000E+00
           3  6.88243E-05  2.88044E-02  6.72958E+01  1.81100E-04  0.00000E+00
           4  0.00000E+00  0.00000E+00  5.01858E-04  1.67284E+01  5.73005E-02
           5  0.00000E+00  0.00000E+00  0.00000E+00  9.24182E-02  2.16993E+01
           6  0.00000E+00  0.00000E+00  0.00000E+00  5.09316E-05  1.55619E+00
           7  0.00000E+00  0.00000E+00  0.00000E+00  2.88608E-06  1.79894E-05

   P0 To Grp  From Grp  6  From Grp  7
           1  0.00000E+00  0.00000E+00
           2  0.00000E+00  0.00000E+00
           3  0.00000E+00  0.00000E+00
           4  0.00000E+00  0.00000E+00
           5  3.77630E-01  0.00000E+00
           6  5.68718E+02  1.29244E+01
           7  1.73726E+01  1.67592E+02
```

Figure 1. Sample Output of ISOTXS Data from the WIMS-ANL Code

Libraries for WIMS-ANL

The variable dimensioning in the WIMS-ANL code removed any size limitation on the number of energy groups for cross section libraries and the development of a version of the NJOY code that can process ENDF/B-VI data have combined to make it possible to generate new libraries. New libraries have now been generated with both 69 and 172 energy groups based on ENDF/B-VI data. The libraries (including the earlier ENDF/B-V based library) have I-135 and Pm-149 added as precursors of

Xe-135 and Sm-149, respectively. The burnup decay chains now also include Pu-238 and Np-237. These added actinides become important at high burnup. Each library includes a secondary data file.

The 69 energy group ENDF/B-VI library matches the group structure of the earlier ENDF/B-V library. The expanded 172 group structure was chosen to also provide library data for the DRAGON code. This library increases the number of energy groups in the resonance range for 13 to 47 and the number of thermal groups from 48 to 80 compared to the 69 group structure. The WIMS-ANL code includes the Segev method for resonance integral interpolation as an option but otherwise has no other revisions in the original resonance treatment.

Each of the libraries available for the WIMS-ANL code has about 123 isotopes and with few exceptions identical isotope labels. This makes it easy to run comparison cases with few changes to the input. Some comparisons are provided in the following section.

Comparisons

The earlier versions of the code and the ENDF/B-V library were subjected to comparisons with both Monte Carlo and experiments. Here we provide comparisons with some of these data from this work and the results from the WIMS-ANL code. The results with the various choices for cross section library data are also compared. Since the earlier results were all run using a UNIX workstation, all of the WIMS-ANL results are from a UNIX workstation version unless otherwise noted.

In Table I the WIMS-ANL code results are compared with the earlier WIMS and VIM Monte Carlo[7] results for the IAEA benchmark standard fuel assembly with LEU fuel. ENDF/B-V based data is used in each case. The model in each case is a super-cell with a fourth moderator region. The reaction rate results for WIMS-ANL give slightly better agreement with VIM for Al, H and U-238 but slightly worse agreement for U-235. The comparison of the k-infinity values have both the WIMS-ANL and the WIMS-D4M values higher than that predicted by VIM. In each case the agreement with Monte Carlo is still quite good, and the WIMS-ANL and WIMS-D4M results are almost identical.

Table I. Relative Absorption Rate and K-infinity Data for IAEA Standard LEU Fuel Assembly

Isotope	WIMS-ANL	WIMS-D4M	VIM Monte Carlo
U-235	0.8042	0.8037	0.8018
U-238	0.0811	0.0804	0.0837
Al	0.0348	0.0351	0.0348
O	0.0022	0.0022	0.0022
H	0.0769	0.0772	0.0770
Si	0.0008	0.0008	0.0008
k-infinity	1.6409	1.6400	1.6356 $\pm$0.0005
Difference, %	+0.197	+0.164	---

The next set of data compares both WIMS-ANL and MCNP4B Monte Carlo[8] with the critical sphere benchmark ORNL-10. The results with 69 group ENDF/B-V data and with 69 and 172 group ENDF/B-VI data are shown in Table II. MCNP4B uses continuous energy ENDF/B-V and -VI based data. The agreement between WIMS-ANL and MCNP4B for an infinite medium is good with version VI data giving better agreement. Earlier comparisons with ENDF/B-V data gave a VIM estimate of 1.0722 $\pm$0.0005, which compares more favorably with the current WIMS-ANL value. The critical estimates in Table II are for DIF3D[9] using the WIMS-ANL generated microscopic data. Again the

agreement improves with version VI data for both DIF3D and MCNP4B. DIF3D with 69 group library data is over predicting critical by 0.26%, while MCNP4B is predicting almost the exact value. The DIF3D prediction with 172 group data is slightly better at 0.20%.

Table II. Comparisons with the ORNL-10 Critical Sphere Benchmark

	k-infinity		Critical	
ENDF/B (Groups)	**WIMS-ANL**	**MCNP4B**	**WIMS-ANL**	**MCNP4B**
V (69)	1.0720	1.0741 ±0.0004	1.00402	1.00429 ±0.0010
VI (69)	1.0707	1.0717 ±0.0005	1.00266	0.99936 ±0.0012
VI (172)	1.0705	1.0717 ±0.0005	1.00202	0.99936 ±0.0012

The following series of tabulated data compare the k-infinity and selected cross section data for the three libraries using the IAEA benchmark simple LEU unit cell. The WIMS-ANL microscopic cross sections are all in a seven energy group set with the energy boundaries shown in Table III. The 172 group set has slightly different boundaries as shown with the largest difference being in the upper bound for the highest energy group. The lower energy cut off also differs with 1.000E-05 eV for the 69 group sets and 1.100E-04 eV for the 172 group set.

Table III. Energy Boundaries for Broad Group Cross Section Data

	Upper Energy Boundary, eV	
Group	**69 Group Data**	**172 Group Data**
1	1.000E+07	1.964E+07
2	8.210E+05	8.208E+05
3	5.530E+03	5.531E+03
4	4.000E+00	4.000E+00
5	6.250E-01	6.250E-01
6	2.500E-01	2.480E-01
7	5.800E-02	5.800E-02

The microscopic cross section data for U-235 fission, U-238 capture and Pu-239 fission are given in Tables IV, V and VI, respectively. Table IV also shows the cell k-infinity values. The largest differences, as one might expect, are between the different ENDF/B versions. The differences between the 69 and 172 group data for version VI are small and distributed among all of the energy groups, i.e. no one energy range appears to dominate. The impact of a 172 energy group library on full reactor computations has not been thoroughly studied at this time.

Table IV. U-235 Microscopic Fission Cross Sections and K-infinity

Group	V (69)	VI (69)	VI (172)
1	1.26421E+00	1.24327E+00	1.24497E+00
2	1.64806E+00	1.65350E+00	1.64904E+00
3	2.29576E+01	2.25591E+01	2.26248E+01
4	3.69821E+01	3.62886E+01	3.62687E+01
5	1.26964E+02	1.27426E+02	1.28034E+02
6	2.48981E+02	2.52056E+02	2.50892E+02
7	5.48027E+02	5.53165E+02	5.53078E+02
k-infinity	1.66303	1.66164	1.66128

Table V. U-238 Microscopic Capture Cross Sections

Group	V (69)	VI (69)	VI (172)
1	5.45110E-02	5.56407E-02	5.57064E-02
2	2.64615E-01	2.56151E-01	2.55076E-01
3	8.69832E+00	8.64062E+00	8.68246E+00
4	5.17347E-01	5.20533E-01	5.20495E-01
5	7.26854E-01	7.30444E-01	7.31746E-01
6	1.33702E+00	1.34424E+00	1.33862E+00
7	2.55246E+00	2.58527E+00	2.58488E+00

Table VI. Pu-239 Microscopic Fission Cross Sections

Group	V (69)	VI (69)	VI (172)
1	1.90013E+00	1.89749E+00	1.89999E+00
2	1.65714E+00	1.62658E+00	1.62747E+00
3	2.68387E+01	2.69183E+01	2.71096E+01
4	2.91822E+01	2.83055E+01	2.83180E+01
5	1.19426E+03	1.19251E+03	1.20860E+03
6	5.64438E+02	5.64391E+02	5.65421E+02
7	7.07905E+02	7.16914E+02	7.16801E+02

Tables VII and VIII show the variation in k-infinity and cross section data with burnup and with the use of different processors, operating systems and compilers. The operating systems include UNIX, Windows 95 and NT and Linux on PC. The compiler for UNIX is the Solaris SUNWspro 4.2, the Windows compilers are Lahey LF90 and F77L, and the Gnu compiler is used with Linux. All PC applications use Pentium II processors. While the initial k-infinity values are identical, the systems each show some drift in the data at higher burnups. The differences are small and not divergent. The differences in the microscopic cross sections generated with burnup are small. It has not been possible to trace the contributions to individual differences in floating point processors, compiler treatments, etc., but it is probably a combination of all of these.

Table VII. K-infinity with Burnup for Assorted Operating Systems, Processors and Compilers

	K-infinity Data			
Burn Step	**UNIX Solaris Compiler**	**Windows NT LF90 Compiler**	**Windows 95 F77L Compiler**	**Linux G77 Compiler**
0	1.66303	1.66303	1.66303	1.66303
1	1.66281	1.66281	1.66282	1.66282
2	1.59322	1.59322	1.59391	1.59391
3	1.56006	1.56004	1.56189	1.56250
4	1.53528	1.53445	1.53572	1.53642

Table VIII. Variation in Cross Section Data with Computers, Compilers and Burnup

	U-235 Fission Cross Sections at Burn Step 4			
Group	**UNIX Solaris Compiler**	**Windows NT LF90 Compiler**	**Windows 95 F77L Compiler**	**Linux G77 Compiler**
1	1.26425E+00	1.26425E+00	1.26426E+00	1.26426E+00
2	1.64819E+00	1.64819E+00	1.64818E+00	1.64818E+00
3	2.31030E+01	2.31031E+01	2.30973E+01	2.30973E+01
4	3.69517E+01	3.69518E+01	3.69547E+01	3.69547E+01
5	1.26658E+02	1.26658E+02	1.26664E+01	1.26665E+02
6	2.49441E+02	2.49426E+02	2.49351E+02	2.49363E+02
7	5.51210E+02	5.51192E+02	5.51006E+02	5.51021E+02

Conclusions

The results of this study show that the WIMS-ANL version, as upgraded, can be used across a variety of machines, compilers and operating systems. This revised code offers the capability of using enriched libraries both in the number of energy groups allowed and in the detailed data now available with a secondary file. The revised FORTRAN makes the code much more easy to read and maintain. The output in addition to being much more readable is under the complete control of the user as to content. The default output settings can be select to fit the tastes of the local user community. The capabilities provided by the Supercell option and the ability to generate cross sections in a number of desired formats make the WIMS-ANL code a very useful application. Although this is not a attempt to completely validate this version of the code, the results here agree well with earlier Monte Carlo and experimental results.

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