



# Development and verification of a 281-group WIMS-D library based on ENDF/B-VII.1



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## ABSTRACT

The WIMS-D library based on WIMS 69 or XMAS 172 energy group structures is widely used in thermal reactor research. Otherwise, the resonance overlap effect is not taken into account in the two energy group structure, which limits the accuracy of resonance treatment. The SHEM 281 group structure is designed by the French to avoid the resonance overlap effect. In this study, a new WIMS-D library with SHEM 281 mesh is developed by using the NJOY nuclear data processing system based on the latest Evaluated Nuclear Data Library ENDF/B-VII.1. The parameters such as the thermal cut-off energy and lambda factor that depend on group structure are discussed. The lambda factor is calculated by Neutron Resonance Spectrum Calculation System and the effect of this factor is analyzed. The new library is verified through the analysis of various criticality benchmarks by using DRAGON code. The values of multiplication factor are consistent with the experiment data and the results also are improved in comparison with other WIMS libraries.

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## 1. Introduction

The WIMS library is used extensively with the WIMS-D code used by many laboratories around the world in the thermal reactor research. The WIMS library with WIMS-D/4 package was processed in the United Kingdom based on the evaluated nuclear data from the 1960s, and there were some problems in this library which have presented in reference Halsall (1991). IAEA initiated the WIMS-D Library Update Project (WLUP) to update working library WIMS-D (Leszczynski, 2007). Several libraries based on group structures WIMS 69 and XMAS 172 were generated as the final product of WLUP, using the evaluated nuclear data from ENDF/B-VI.7, JENDL-3.2, CENDL-3, JEFF-2.2 and ENDF/B-VII.0. To update WIMS-D library, a lot of 69-group cross section libraries were also generated with the recent version of evaluated nuclear data files (Gil et al., 2000; Kim et al., 1989; Rahman et al., 2004). The self-shielding due to elastic resonance is taken into account, and the resonance overlap was treated by weighting flux in the work of Japan Atomic Energy Research Institute (Rahman and Takano, 1996). Furthermore, a computer software package with graphical user interface for MS Windows had been developed at BARC, India (Thiyagarajan et al., 2003).

Since XMAS group structure have been developed to overcome the deficiencies in WIMS group structure (Handbook of Nuclear Engineering, 2010), XMAS group structure is more suitable to calculate MOX fuel and high burn up situations. But it should be noted that XMAS energy group structure does not take into account the resonance overlap effect. SHEM 281 mesh is developed to reduce error due to resonance overlap effect (Handbook of Nuclear Engineering, 2010). It is an effective way to treat resonance overlap effect by multi-group library, and SHEM 281 mesh is chosen.

A new WIMS-D library based on ENDF/B-VII.1 with SHEM 281 mesh is developed to improve the accuracy of assembly calculation using the NJOY nuclear data processing system. In this paper, the method to develop the library is illustrated, and the method calculating lambda factor is also discussed. The accuracy of the library is verified by using series of benchmarks and the results are consistent with the experiment data.

## 2. Development of 281-group WIMS-D library

### 2.1. Data processing method

It is an extremely complex and continuous task to develop a multi-group library. The procedure to develop the WIMS-D library is shown in Fig. 1. The main codes concluding NJOY, WILLIE,

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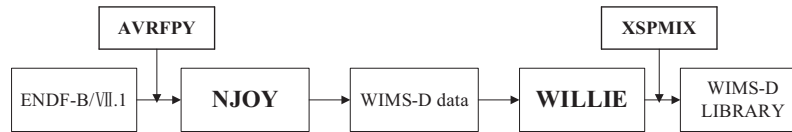


Fig. 1. The flow of WIMS-D library generation.

AVRFPY, and XSPMIX (Leszczynski, 2007) are used. The NJOY nuclear data processing system is a universal code to process the basic evaluated nuclear data into multi-group library or continuous-energy library (MacFarlane et al., 2002). As its comprehensive features and ability to generate the ACE, MATXS and WIMS-D libraries, NJOY is one of most widely used code to process nuclear data.

The modules of NJOY are linked together by input and output files (MacFarlane et al., 2002), and the data flow to generate the WIMS-D library is showed in Fig. 2. The processing task of each module can be found in reference MacFarlane et al. (2002).

WILLIE is a library-maintenance code. The purpose of this code to create a new WIMS-D library, modify an existing library, transform the formatted library into binary or the other way around. And it also can be used as a tool to generate pseudo fission product. The averaged fission spectrum used in the library is calculated by the code XSPMIX. And AVRFPY extracts the fission product yield data in the format of ENDF-6.

## 2.2. Some details of parameters

### (a) Energy group structure

The SHEM 281 mesh is developed to reduce multi-group calculations errors due to resonance overlap effect during 4–22 eV (Santamarina et al., 2008). The resonance overlap effect between  $^{239}\text{Pu}$ ,  $^{241}\text{Pu}$  and  $^{241}\text{Am}$  in 0.26, 0.29, 0.31 eV is paid particularly attention on, and the error of resonance overlap between  $^{235}\text{U}$  and  $^{238}\text{U}$ ,  $^{238}\text{U}$  and  $^{240}\text{Pu}$  is disappeared. Also, other nuclides' resonance peaks are paid attention on.

There are 55 fast groups between 11.14 keV and 20 MeV, 38 resonance groups between 22.5 eV and 11.14 keV, and 118 thermal groups between  $10^{-5}$  eV and 22.5 eV in the library. It is clear that the self-shielding treatment starts at 22.5 eV, which is different from the general that the uppermost energy boundary of thermal energy groups is 4 eV, in that a fined mesh is developed in the 4–23 eV energy ranges and the main resonances are optimization. The multi-group cross sections are plotted to investigate the resonances at 6.67 eV and 20.87 eV of  $^{238}\text{U}$ , and Fig. 3 shows that the SHEM 281 mesh can represent the resonance explicitly and the approximation is small. The calculation also shows that to change the cutoff at 22.5 eV does not introduce significant error and the thermal cut-off energy is suitable.

### (b) Goldstein–Cohen $\lambda$ factor

The Goldstein–Cohen  $\lambda$  factor (lambda factor) is relied on the energy group structure and the uppermost boundary of thermal energy groups (Handbook of Nuclear Engineering, 2010). A method to calculate Goldstein–Cohen  $\lambda$  factor is introduced in reference Leszczynski (1997). The primary idea is to find the relationship between a mixture of refer-

ence resonance nuclide (usually  $^{238}\text{U}$ ) with hydrogen and a mixture of other resonance nuclide, which its  $\lambda_i$  is need to be calculated, with hydrogen (Leszczynski, 1997). Then, the  $\lambda_i$  can be calculated by solving the equation  $\sigma_{b,\text{hom}} = \sigma_{b,\text{het}}$ :

$$\lambda_i = \frac{\sigma_{b,\text{hom}} - N_h \cdot \sigma_{ph}/N_r - \lambda_r \cdot \sigma_{pr}}{N_i \cdot \sigma_{pi}/N_r}$$

where  $\sigma_{pr}$ ,  $\sigma_{ph}$ ,  $\sigma_{pi}$  are the respective potential scattering cross section of the resonance isotope, hydrogen and non-resonance isotope,  $N_r$ ,  $N_h$ ,  $N_i$  are the respective atomic number densities,  $\sigma_{b,\text{hom}}$ ,  $\sigma_{b,\text{het}}$  are the respective dilution cross section of the homogeneous and heterogeneous systems.

Neutron Resonance Spectrum Calculation System (NRSC) Leszczynski, 1997 is used to calculate lambda factor. The lambda factors of  $^{16}\text{O}$ ,  $^{27}\text{Al}$ ,  $^{56}\text{Fe}$ ,  $^{91}\text{Zr}$  are calculated, and other nuclides' are obtained by cubic spline interpolation. The two sets of 1-group lambda factor data for all nuclides in function of the atomic weight are showed in Fig. 4. And the lambda factor for SHEM 281 mesh named factor-b is calculated, which the self-shielding treatment starts at 22.5 eV, while factor-a is based on the WIMS 69 mesh. It is the fact that the cross sections in low energy region show resolved resonances and in high energy region show unresolved resonances, so lambda factor is increasing with the increase of the uppermost boundary of thermal energy groups.

### (c) Averaging spectrum and fission spectrum

The standard PWR spectrum (iwt = 4, or iwt = -4). Note that iwt is weighting spectrum parameter in NJOY code (MacFarlane et al., 2002)) and mid-life PWR spectrum (iwt = 5, or iwt = -5) are the better choices when a library is developed for the thermal reactor. A new spectrum was obtained in WLUP (Leszczynski, 2007), which is more accurate via analysis.

Only one fission spectrum is available in the WIMS library. Integral validation shows that the fission spectrum has no strong effect on integral parameters (Ping, 2001). It's convenient to calculate both the UOX and MOX fuel using the same library, so the fission spectrum is composed of  $^{235}\text{U}$ ,  $^{238}\text{U}$ ,  $^{239}\text{Pu}$  and the weights are 54%, 8%, and 38%, respectively.

### (d) Other parameters

The anisotropic scattering effect has significant affect in light nuclide. Only four nuclides are given P1 scattering matrix (1-H-H<sub>2</sub>O, 1-D-D<sub>2</sub>O, 6-C-nat, 8-O-nat). And the transport cross section is corrected by P1 scattering matrix.

Gadolinium and tungsten are used as burnable materials in AP1000 reactor. These material are paid attention on when material processing, especially tungsten, but there are not suitable benchmarks to validate them yet.



Fig. 2. The data flow in NJOY.

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