Multi-group cross section library generation for HTGR lattice physics code XPZ

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Abstract. The XPZ code was previously developed for the lattice physics computation in High Temperature Gas-cooled Reactors (HTGRs), which adopted the multi-group cross section library converted from the existing open-source DRAGON library. In this paper, a new format of multi-group cross section library named XPZLIB has been implemented in XPZ code. XPZLIB is designed in binary and HDF5 formats, including detailed data contents for resonance, transport and depletion calculations. A new data-processing module named XPZR is developed based on NJOY-2016 to generate nuclide dependent XPZLIB from the most recent evaluated nuclear data, and besides, the PyNjoy-2016 system is developed for automatic generation of integrated XPZLIB including a complete set of nuclides. The new generated XPZLIB is presented with the XPZ code. Numerical results demonstrate the accuracy of the new library XPZLIB and the reliability of the data processing scheme. Moreover, the influence of different versions of ENDF/B data is investigated.

1. Introduction

The multi-group cross section library is the basis and prerequisite for the lattice physics calculation of neutron transport in reactor analyses. The library can provide all kinds of different nuclear data, including nuclides properties, temperature-dependent cross sections, burnup information and some other related quantities required by lattice physics computations. Therefore, the accuracy of a lattice physics code can be significantly influenced by the multi-group cross section library [1]. The multi-group cross section library utilized directly by the lattice code is processed from the evaluated nuclear data library by using the specific data processing code. The ENDF/B [2] library established by the American Cross Section Evaluation Working Group (CSEWG) is the most comprehensive and widely used evaluated nuclear data library around the world. The NJOY nuclear data processing system developed by Los Alamos National Laboratory (LANL) is a computer code package that uses a modular program structure to produce pointwise and multi-group nuclear cross sections and other quantities from evaluated nuclear data [3].
Most lattice physics codes have their own multi-group cross section libraries. For instance, WIMS developed through various versions at the UK laboratory AEE/Winfirth uses the library WIMSLIB [3]. WIMSLIB is developed continuously by a Co-ordinated Research Project (CRP) WIMS Library Update Project (WLUP) supported by IAEA [4]. DRAGLIB is a cross section library for lattice code DRAGON which is developed by Polytechnique Montréal [5]. The PyNjoy-2012 system that can simplify the management of all the NJOY runs is a set of Python scripts dedicated to the production of DRAGLIB [6]. In addition to WIMS and DRAGON, many other codes use the MATXS format libraries and corresponding post-processing program to generate dedicated cross section libraries [1][7][8].

In our previous work, the XPZ code was developed for lattice physics calculation, as well as for the generation of broad-group constants [9] in High Temperature Gas-cooled Reactors (HTGRs). XPZ utilized a cross section library converted from the open-source library DRAGLIB. The latter was processed from the ENDF/B-VII.0 nuclear data by NJOY-2012.

This paper introduces a new format of multi-group cross section library named XPZLIB that has been recently implemented in XPZ code. The new library is processed from the ENDF/B data by developing a new data-processing module named XPZR in the open-source NJOY-2016 code. Besides, a processing system PyNjoy-2016, based on PyNjoy-2012, is developed to realize the automatic generation of multiple sets of XPZLIB.

The remainder of the paper is organized as follows. Section 2 introduces the format and characteristics of XPZLIB as well as generation flow and scheme of XPZR. Numerical results of critical and burnup calculations based on produced libraries are presented for validation in Section 3. Finally, concluding remarks are given in Section 4.

2. Generation of the Multi-group Cross Section Library

2.1. XPZLIB Format and Characteristics

XPZLIB has two types of formats: binary format and HDF5 format [10].

Binary format XPZLIB consists of four basic data files, i.e., NUCLIDES, XSDIR, DEPL_CHAIN and ENERGY.

The NUCLIDES file contains one- and two- dimensional cross sections of all nuclides. As a binary file, it can save storage space and realize fast reading. Since the microscopic cross sections stored in a cross-section library are usually dependent on the background cross section and temperature [11], the format of the file is organized in multi-loop structure. As is shown in Table 1, the structure includes the nuclide loop, the temperature loop and the dilution loop from the outside in. And the NUCLIDES file structure is shown in Fig. 1.

The XSDIR file stores the list of nuclides and the address of data blocks in the NUCLIDES file for each nuclide, which is used for fast data access. The DEPL_CHAIN file contains the depletion chains used for burnup calculations. The ENERGY file is used to describe the energy group structure.

Although the binary format can realize fast reading and storage space saving, the users cannot read and look up the specific nuclear data directly. In order to maintain the advantages of binary format and make it convenient to look up nuclear data, XPZR is developed to generate the library in a HDF5 format. The HDF5 format library has only one file: NUCLIDES.h5. The file contains cross sections of all nuclides in multi-loop structures as the same as the binary format, energy group structure and depletion related data.

| LOOP | Parameter          |
|------|--------------------|
| 1    | Nuclide-e.g. U235  |
| 2    | Temperature-e.g. TMP00XX |
| 3    | Background XS-e.g. BGXS00XX |
The data contents comprised in XPZLIB are as detailed as DRAGLIB, which is well suited for general fission reactors. For example, the XPZLIB processed from ENDF/B-VII.0 using SHEM-361 energy structure is summarized as follows:

- Evaluated nuclear data libraries: ENDF/B-VII.0;
- Number of nuclides: 314;
- Number of fissile nuclides: 31;
- Number of heavy nuclides: 42;
- Number of fission fragments: 272;
- Number of resonance nuclides: 68;
- Energy group structure: SHEM-361;
- Energy range: $1.964 \times 10^{-7}$-$1.100 \times 10^{-5}$ eV;
- Range of resonance energy groups and energy: 31-173 group, $3.2065 \times 10^{5}$-$22.536$ eV; 52-173 group, $1.8585 \times 10^{4}$-$22.536$ eV;
- $S(\alpha, \beta)$ data: including all important available $S(\alpha, \beta)$ materials in ENDF/B data, such as H in H$_2$O, C in graphite, etc.;
- Maximum Legendre order: P1;
- Temperatures: typically including five temperature grid points, i.e., 293.0K, 550.0K, 900.0K, 1200.0K, and 2000.0K;
- Background cross sections: The number of background cross sections for most resonance nuclides is limited to less than or equal to 10, but for the following nuclides that have a considerable resonance effect, it is 20, including $^{232}$Th, $^{235}$U, $^{238}$U, $^{239}$Pu, $^{240}$Pu, $^{241}$Pu, $^{242}$Pu and $^{241}$Am;
- Reactions or quantities dependent on temperature: (n, tot), (n, n) (n, n'), (n, 2n), (n, 3n), (n, 4n), (n, f), (n, np), (n, γ), (n, p), (n, d), (n, t), (n, α), (n, 2α), $\nu \sigma_f$ (neutron number per fission multiply fission cross section), fission spectrum and scattering matrix;
- Reactions or quantities dependent on background cross section: (n, tot), (n, n), (n, f), (n, γ), $\nu \sigma_f$ and scattering matrix;
- Depleting channels: (n, 2n), (n, 3n), (n, 4n), (n, f), (n, np), (n, γ), (n, p), (n, d), (n, t), (n, α), (n, 2α) and radioactive decay.

Figure 1. The NUCLIDES file structure.
2.2. *XPZLIB Generation Flow and Scheme*

The generation flow of XPZLIB is presented in Fig. 2. The ENDF/B data are processed by NJOY-2016. Several modules are available to process the cross-section data from neutron sub-library of ENDF/B. The specific modules are as follows: MODER, RECONR, BROADR, UNRESR, THERMR and GROUPR. After processing from module GROUPR, the output file is in GENDF format [3], which is further processed by the post-processing module XPZR. The XPZR module performs the final conversion from GENDF format towards XPZLIB format.

![Flow chart of XPZLB generation.](image)

The development of XPZR is based on DRAGR module in NJOY-2012 [13]. XPZR has two functions: one is to provide available data required by XPZ from GENDF files and the other is to generate the depletion file from decay and neutron fission yield sub-libraries of ENDF/B.

An important issue is the generation of fission-related data, i.e., fission spectrum and $\nu \sigma_f$ values. The following equations are used [13] [11] in XPZR.

$$\chi_g = \frac{\sum_g \sigma_{f,g} \rightarrow g \Phi_g + \chi_{d,g} \sum_g \nu_{d,g} \sigma_{f,g} \Phi_g}{\sum_g \sum_g \sigma_{f,g} \rightarrow g \Phi_g + \sum_g \nu_{d,g} \sigma_{f,g} \Phi_g} \quad (1)$$

$$\nu g \sigma_{f,g} = \sum_g \nu_{d,g} \sigma_{f,g} \rightarrow g + \nu_{d,g} \sigma_{f,g} \quad (2)$$

$$\chi_{d,g} = \frac{\sum_g \nu_{d,g}}{\sum_g \nu_{d,g}} \quad (3)$$

where,

$\chi_g$: fission spectrum,

$\chi_{d,g}$: fission spectrum of delayed neutron,

$\sigma_{f,g} \rightarrow g$: fission matrix,

$\sigma_{f,g}$: fission cross section,

$\nu g$: number of neutrons generated by a fission,

$\nu_{d,g}$: number of delayed neutrons generated by a fission,

$\phi_g$: weighting flux.
The scattering matrix can be obtained by the following equation [13] in XPZR:

$$\sigma_{\text{scat}, g' \rightarrow g} = \sigma_{\text{diffusion}} + \sigma_{n2n, g' \rightarrow g} + \sigma_{n3n, g' \rightarrow g}$$  \hspace{1cm} (4)

where,

- $\sigma_{\text{scat}, g' \rightarrow g}$: scattering matrix,
- $\sigma_{\text{diffusion}}$: diffusion matrix,
- $\sigma_{n2n, g' \rightarrow g}$: (n, 2n) reaction matrix,
- $\sigma_{n3n, g' \rightarrow g}$: (n, 3n) reaction matrix.

Above the thermal cut-off energy, the static scattering matrix including elastic and inelastic scattering is used as the diffusion matrix. In the thermal energy range, coherent and incoherent scattering matrix is requested as the diffusion matrix.

To reduce the storage requirement of the scattering matrix, XPZR uses the same sparse-matrix storage approach as in MATXSR module [3].

In thermal energy range, the total cross sections need to be modified. Specifically, the static scattering cross section is deducted from the total cross section and the corresponding thermal scattering cross sections including coherent and incoherent thermal scattering are added to the total cross sections.

As for burnup data, XPZR inherits the lumped fission product treatment [14] from DRAGR, which removes those nuclides that have very short half-lives and small fission yields.

2.3. Automated Generation System PyNjoy-2016

The processing system PyNjoy-2016 is developed for automatic generation of XPZLIB containing a complete set of nuclides. The system is made of three components: the NJOY-2016 program including post-processing module XPZR, a generic Python script PyNjoy.py and a collection of Python datasets.

As is shown in Fig.3, in the system, the Python script, named PyNjoy.py, has been used to define corresponding functions to prepare input files required by NJOY modules automatically, and then to execute the modules in correct order. As for Python datasets, firstly, they can define parameters of all nuclides, which are used during processing, such as temperature, background cross section, Legendre order, energy group structure and so on. Secondly, the datasets can import functions in PyNjoy.py to execute NJOY-2016 to process a large number of nuclides in the defined directory.

![Figure 3. The generation flow of PyNjoy-2016 system.](image)

The specific generation flow is shown in Fig. 4: the function `self.pendf()` is used to process the ENDF-6 format file to PENDF format file; the function `self.gendf()` is used to process PENDF format file to GENDF format file; the function `self.xpzlib()` can process the GENDF format file to XPZLIB; and besides, the function `self.burnup()` can process the burnup data.
3. Numerical Validation and Analyses

3.1. Numerical Validation

In order to validate the processed XPZ libraries, the realistic fuel pebble in HTR-10 reactor [15] is calculated. The HTR-10 fuel pebble model is shown in Fig. 5. The pebble consists of the fuel zone and the graphite shell, having the radius of 2.5 cm and 3.0 cm, respectively. And the fuel zone is filled with dispersed fuel particles. The dispersed particle with four coated layers is shown in Fig. 6.

Table 2 and 3 give the parameters of the realistic HTR-10 fuel ball and coated fuel particle [15].

| Table 2. HTR-10 Pebble fuel element characteristics. |
|------------------------------------------------------|
| Diameter of ball (mm)                               | 60  |
| Diameter of fuel zone (mm)                          | 50  |
| Density of graphite in matrix and outer shell (g/cm³) | 1.73|
| Heavy metal (U) loading per ball (g)                | 5.0 |
| Enrichment of $^{235}$U                             | 17% |
| Equivalent natural boron contents of impurities in uranium | 4 ppm|
| Equivalent natural boron contents of impurities in graphite | 1.3 ppm|
| Volumetric filling fraction of coated fuel particle in the fuel zone | 0.05|
Table 3. Coated fuel particle characteristics.

| Layer radius (mm) | Material | Density (g/cm³) |
|------------------|----------|----------------|
| 0.25             | UO₂      | 10.4           |
| 0.34             | PyC      | 1.1            |
| 0.38             | PyC      | 1.9            |
| 0.415            | SiC      | 3.18           |
| 0.455            | PyC      | 1.9            |

The HTR-10 pebble model is calculated by XPZ adopting the old library and the new XPZLIB, respectively. The Mont Carlo code OpenMC [16] developed by Massachusetts Institute of Technology is taken as the reference code, which uses an HDF5-format continuous cross section library. All libraries are based on the same evaluated nuclear data library ENDF/B-VII.0. The calculation results of OpenMC have standard deviations being 10⁻⁴ magnitude. Table 4 and 5 provide the $k_{eff}$ calculation results. It is seen that the $k_{eff}$ results of XPZ based on new XPZLIB show very good agreement with the results based on the old library, with only a few pcm differences between each other. Besides, the differences between XPZ and OpenMC are in an acceptable range.

Table 4. $k_{eff}$ calculation results of XPZ based on old library and new XPZLIB.

| Filling ratio | Old Lib | New Lib | Difference (PCM) |
|---------------|---------|---------|------------------|
| 5.025%        | 1.691781| 1.691780| -0.1             |
| 10.049%       | 1.543318| 1.543312| -0.6             |
| 20.099%       | 1.355486| 1.355481| -0.5             |

Table 5. $k_{eff}$ calculation results of OpenMC and XPZ based on new XPZLIB.

| Filling ratio | OpenMC | XPZ     | Difference (PCM) |
|---------------|--------|---------|------------------|
| 5.025%        | 1.69124| 1.691780| 54.0             |
| 10.049%       | 1.54485| 1.543312| -153.8           |
| 20.099%       | 1.35547| 1.355481| 1.1              |

Figure 7. HTR-10 fuel ball burnup calculation results based on old library and new XPZLIB.
Burnup calculations are performed for a more comprehensive validation of the XPZLIB, especially for the burnup data. In the test, the filling ratio is 5.025% and the power density is 90W/gU. Fig. 7 shows dependence of $k_{eff}$ on burnup in HTR-10 pebble. The result based on old library is regarded as the reference data. The difference at every burnup step is within 5 pcm, which demonstrates the accuracy of the new library XPZLIB and the reliability of the data processing scheme.

3.2. Comparisons on different versions of ENDF/B data

Table 6 gives the $k_{eff}$ results calculated by XPZ based on ENDF/B-VII.0, ENDF/B-VII.1 and ENDF/B-VIII.0. It is found that version of evaluated nuclear data file can make a big influence on the results. The old library is processed from ENDF/B-VII.0. After updating the evaluated nuclear data library to ENDF/B-VIII.0, the result values will decrease by about 0.3%-0.6%.

| Filling ratio | XPZ VII.0 | XPZ VII.1 | XPZ VIII.0 |
|---------------|-----------|-----------|------------|
| 5.025%        | 1.691780  | 1.686013  | 1.681245   |
| 10.049%       | 1.543312  | 1.540592  | 1.536338   |
| 20.099%       | 1.355481  | 1.354254  | 1.351402   |

In addition to $k_{eff}$ calculation, Fig. 8 gives the burnup calculation results based on different evaluated nuclear data libraries. The result based on ENDF/B-VII.0 is considered as the reference. Then, it can be seen that there exist about 0.3%-0.5% differences between ENDF/B-VII.0 and ENDF/B-VII.1, while 0.5%-0.7% differences between ENDF/B-VII.0 and ENDF/B-VIII.0. It is noted that all the above XPZ calculation results based on binary format is almost the same as HDF5 format, which the difference is within 0.2 pcm.

![Figure 8. HTR-10 fuel ball burnup calculation results based on different evaluated nuclear data libraries.](image)

4. Conclusions

This paper introduces the development of the XPZR module in NJOY-2016 to generate the multi-group cross section library XPZLIB for lattice physics code XPZ. Numerical results demonstrate the accuracy of the new library XPZLIB and the reliability of the data processing scheme. Comparison studies on different versions of ENDF/B data are also presented, which will be further investigated in our future work.
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