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Study on processing and validation of ENDF/B-VIII nuclear data library by criticality benchmark of PWR pin cells using NJOY21 and OpenMC

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ABSTRACT

Nuclear reaction cross section is a key factor in Monte Carlo simulation of various reactor physics calculation including material properties and geometry. For various purposes including radiation dosimetry, shielding calculation and criticality calculation of reactor physics different organizations produce different nuclear data library such as ENDF, JEFF, JENDL, CENDL, TENDL etc. Different formats of these data libraries - ENDF-6, ACE, hdf5 are available for use in different reactor physics codes. Different types of deterministic and stochastic reactor physics code like MCNP, Serpent, WIMSD, OpenMC are available for criticality calculation. In this study, an open-source Monte Carlo particle transport code OpenMC was used to calculate the criticality of UO_2 and $UPuO_2$ fueled PWR pin cells. JEFF-3.2 and ENDF/B-VIII continuous energy cross-sections data libraries were used with OpenMC to perform the criticality calculations. Raw nuclear data of ENDF/B-VIII library, released on February 28, 2017, was processed and transformed into ACE format by using latest NJOY21 data processing code. Quality assurance procedures have been applied to ensure the ENDF/B-VIII processed files. The obtained results on data processing of ENDF/B-VIII library and k_{eff} are analyzed and discussed in this paper.

Keywords: Nuclear data, Neutronics, NJOY21, OpenMC.

1. Introduction

Nuclear data contains energy dependent reaction cross sections, the energy and the angular distribution of neutrons and reaction products for various combination of incident particle and target atoms. It also contains atomic and nuclear properties in excited states and their radioactive decay data. Therefore, these data are essential nuclear power application along with fusion research, shielding calculation, medical, non – destructive testing and environmental monitoring applications [1]. For accurate neutronics simulation available deterministic and Monte Carlo both types of codes depend on most accurate nuclear data for appropriate representation of underlying physical processes.

There are two types of data available experimental nuclear data libraries and evaluated nuclear data libraries. The experimental nuclear data library[2] EXFOR is released by Nuclear Data Center (NDS) of IAEA which is comprehensive compilation of nuclear data from approximately 22000 experiments. EXFOR library contains data of total cross-section, fission cross-section, absorption cross-section, scattering cross-section, double differential cross-section, fission products etc. Most of the time the experimental data is not sufficient for nuclear modeling, to fill the gap between experimental data and application requirements, physics-based models were introduced. Experimental data combined with physics-based models is called evaluated nuclear data. USA, Japan, China, Europe and Russia have developed their own evaluated nuclear data library with large incident energy range for large number of isotopes. Most common data libraries are ENDF/B[3], JEFF[4], CENDL[5], JENDL[6], BROND[7] etc. In this study ENDF/B-VIII[8] which was released in 2018 contains 557 nuclides was processed to use in benchmarking.

Different neutronics codes use different data formats of the evaluated nuclear data library. Deterministic codes like WIMSD, DRAGON etc. use nuclear data in WIMSD[7], MATXS, AMPX formats. On the other hand Monte Carlo codes like MCNP[9], Serpent[10], OpenMC[11] used data in ACE, hdf5 formats. For this various application evaluated data needed to process into continuous energy representation or multigroup representation. To read, convert and process the evaluated data a nuclear data processing code NJOY was introduced. In this study NJOY21[12] data processing code was used to process and convert the evaluated data of ENDF/B-VIII nuclear data library to use it for benchmarking of UO_2 and $UPuO_2$ fueled pincell in an open-source Monte Carlo neutral particle code called OpenMC.

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2. Methods

2.1 Method of data processing

The data processing code NJOY was developed by Los Alamos National Laboratory, USA. The functions of NJOY code are to read evaluated nuclear data in ENDF format, to transform the data in various way, to output the result for various application such as dosimetry, reactor criticality, shielding calculation etc. In this study of evaluated nuclear data processing the workflow of NJOY was begin with conversion of ASCII data file into Binary format and then resonance and reaction reconstruction in point-wise evaluated nuclear data files. The following step was Doppler broadening of data at our desired temperatures and creating point-wise heat production cross-section and producing cross-section and scattering distribution in thermal energy range at the desired temperatures and finally converting the point-wise file into several ACE files depending on the temperature requirements. The data process diagram of NJOY is shown in fig 1.

The NJOY code consists of several modules including moder, reconr, heatr, thermr, gaspr, acer etc. The produced ACE format data can be directly use in MCNP and Serpent Code. But all the ACE files for individual nuclides was combined and converted into single hdf5 format using built-in command of OpenMC. Since all the temperature data of individual nuclide is available in one hdf5 file, it eliminates the use of suffixes in cross-section data, reduces storage requirement[13] for nuclear data and memory requirement during transport simulation and also allows users to mention nuclides and temperatures only in the model.

2.2 Method of Benchmarking

In a Monte Carlo simulation, the three most important requirements are material composition, geometry specification and nuclear cross-section data. All of these requirements was implemented in this benchmarking study through the highly enriched Python API of OpenMC. For the benchmarking and comparison of result the LWR pincell specification was taken from JEFF report 15[14] published by NEA, OCED in September 1999.

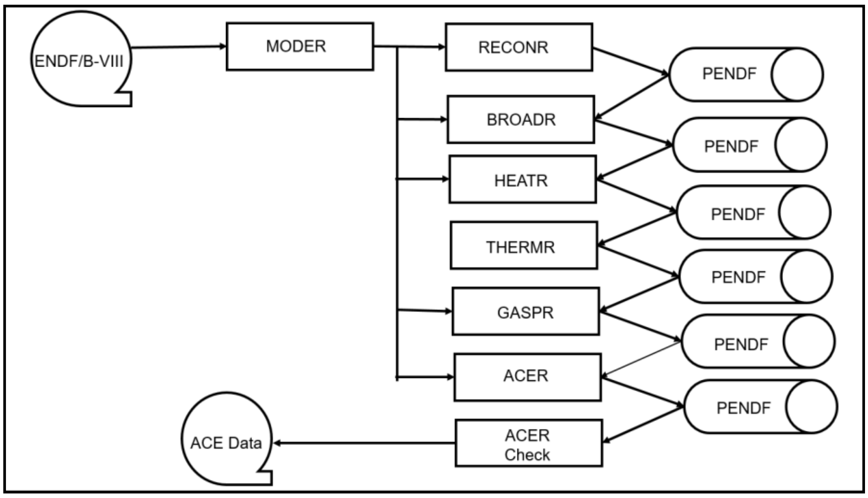

Fig. 1: NJOY data flow diagram

2.3 Material composition

The material compositions of LWR pincell, MOX pincell and geometric configuration of the pincell are shown on table 1 and 2.

Table 1: LWR UOX pincell material composition

Region	Nuclides	Case 1	Case 2, 3, 4
Region 1	U235	0.00070803	0.00070803
	U238	0.022604	0.022604
	O16	0.046624	0.046624
Region 2	Zr	0.043241	0.043241
Region 3	H	0.066988	0.046892
	O16	0.033414	0.023446
Alternatively	H_2O	0.033494	0.023446

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Table 2: LWR MOX pincell material composition

Region	Nuclides	Fuel MOX-1	Fuel MOX-2
Region 1	U235	0.00005105	0.00005118
	U238	0.02037	0.02042
	Pu238	0.00004669	0.00002714
	Pu239	0.001465	0.001972
	Pu240	0.0005691	0.0004256
	Pu241	0.0002713	0.00003577
	Pu242	0.0001413	0.00001234
	Am241	0.00003028	0.00001406
	O	0.04588	0.04588
Region 2	Zr	0.0388	0.0388
Region 3	H	0.04744	0.04744
	O	0.02372	0.02372

2.4 Geometry specification

The UOX and MOX pincell radius and square lattice pitch are shown in table 3.

Table 3: Geometry of UOX and MOX pincell

Region	UOX	MOX
Fuel radius	0.4 cm	0.41 cm
Clad radius	0.45 cm	0.475 cm
Pitch	1.2 cm	1.26 cm

3. Results

NJOY processed data of ENDF/B-VIII nuclear data library compared with JEFF 3.2 showed result with satisfactory agreement. The fission cross-section of U235 and U238 at 293K temperature and elastic scattering cross-section of O16 at 293K temperature from ENDF/B-VIII data compared with JEFF 3.2 data are shown in figure 2 to 4.

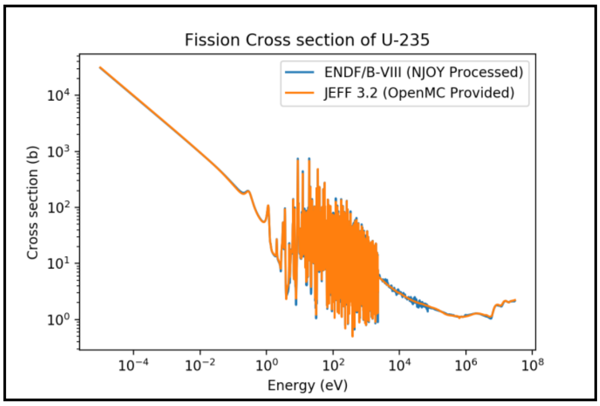

Fig. 2: Fission cross-section of U^{235}

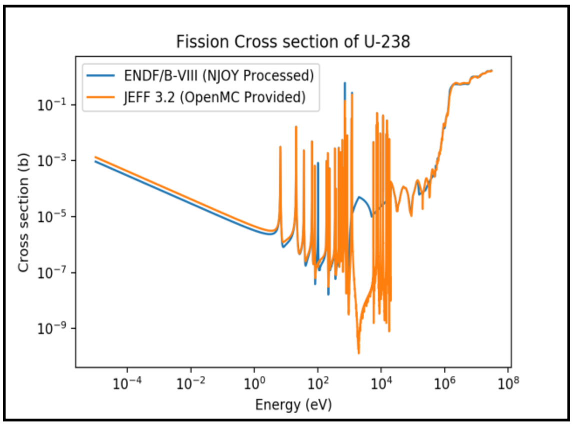

Fig. 3: Fission cross-section of U^{238}

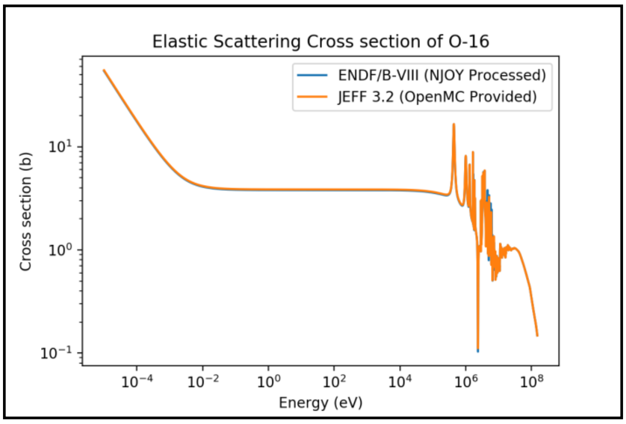

Fig. 4: Elastic scattering cross-section of O^{16}

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The cross –section comparison of the nuclides between JEFF-3.2 data and NJOY21 processed ENDF/B-VIII data showed good agreement with few deviations in the resonance range which suggest that the processing of data was correct.

To calculate the multiplication factor and flux of the pincell the computational domain or pincell geometry created by Python API of OpenMC is shown in fig 5.

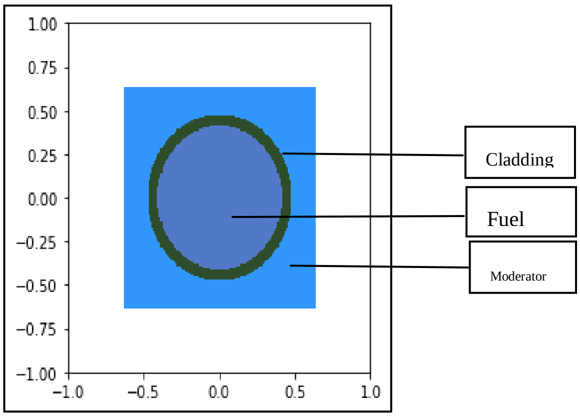

Fig. 5: Pincell

The UOX pincell K-inf value computed with NJOY processed ENDF/B-VIII data and JEFF 3.2 data library and compared with other codes is shown in table 4. The simulation was done in 400 active batches and 50 inactive batches with 50,000 particles in each batches. For UO_2 pincell the simulation was done in 4 cases, isothermal case – where fuel, cladding and moderator all are in 293K temperature, the reduced density isothermal case – where the temperature is 293 but moderated density is 0.7 times of previous case, the third case is different temperature for each region – fuel at 900K, cladding at 600K and moderator at 550K and the fourth case is again isothermal where all regions are at 550K temperatures. The k_{eff} of UO_2 pincell for all cases compared with other codes is presented in table 4.

The K_{eff} of MOX pincell for various cases is shown in table 5.

Table 4: UOX pincell K-inf result compared with other codes

Code with version	Case 1 Isothermal (All region 293K)	Case 2 Isothermal (All region 293K) Reduced moderator density	Case 3 Fuel at 900K, Clad at 600K, Moderator at 550K	Case 4 Isothermal (All region 550K)
MCNP-4A (Petten)	1.39011 (±0.00040)			1.31492 (±0.00040) (from cylindrical geometry)
MCNP-4B (Cadarache)	1.38979 (±0.00007)			
MCNP-4A (Stuttgart)	1.38994 (±0.00060)	1.33827 (±0.00060)	1.30678 (±0.00060)	
MONK-7 (Winfrith)	1.38910 (±0.00010)			
TRIPOLI-4 (Cadarache)	1.38849 (±0.00018)			1.31539 (±0.00087) (from cylindrical geometry)
OpenMC 0.10.0 (JEFF 3.2)	**1.38838 (±0.00061)**	**1.33625 (±0.00035)**	**1.30264 (±0.00064)**	**1.31554 (±0.00092)**
OpenMC 0.11.0 ENDF/B-VIII	**1.38601 (±0.00021)**	**1.33296 (±0.00031)**	**1.30090 (±0.00047)**	**1.31457 (±0.00046)**

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Table 5: MOX pincell K-inf result compared with other codes

Code	MOX 1		MOX 2	
Temperature	Fuel at 300K	Fuel at 560 K	Fuel at 300K	Fuel at 560 K
MCNP (Stuttgart)	1.2270 (±0.00031)	1.2127 (±0.00050)	1.2692 (±0.00040)	1.2553 (±0.00030)
MONK-7 (Winfrith)	1.2260 (±0.00050)		1.2686 (±0.00050)	
MORSE-K (Stuttgart)	1.2237 (±0.00080)	1.2100 (±0.00080)	1.2652 (±0.00080)	1.2524 (±0.00080)
APOLLO-2.4.1	1.22723	1.21242	1.26876	1.25485
SCALE-4.2/KENO	1.2279 (±0.00020)	1.2137 (±0.00020)	1.2701 (±0.00020)	1.2562 (±0.00020)
OpenMC – 0.10.0 JEFF 3.2	**1.22796 (±0.00064)**	**1.21372 (±0.00060)**	**1.27813 (±0.00065)**	**1.26377 (±0.00062)**
OpenMC – 0.11.0 ENDF/B-VIII	**1.23493 (±0.00061)**	**1.21894 (±0.00061)**	**1.28174 (±0.00070)**	**1.26657 (±0.00054)**

The normalized flux profiles of UO_2 and $UPuO_2$ are shown in figure 6 and 7.

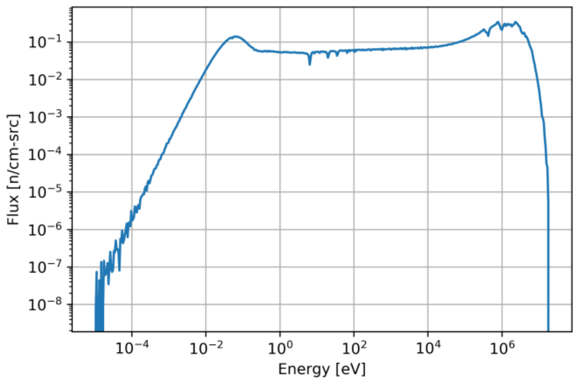

Fig. 6: Normalized flux profile of UOX pincell

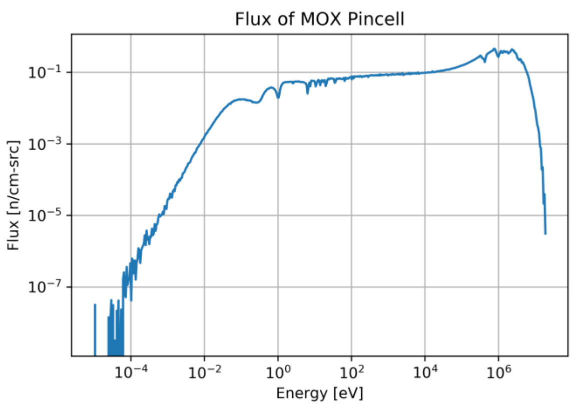

Fig. 7: Normalized flux profile of MOX pincell

In both normalized flux plots, the thermal energy region is 10^{-5} eV to 0.625 eV and beyond that is fast energy region. The neutron flux unit here is neutron per cm-source. It can be converted to neutron/cm^2-sec by multiplying the normalization factor.

4. Conclusion

Nuclear data is one of the key factor in neutronics simulation. The transformation of evaluated data at required temperatures and use it in simulation yields in more accurate result than the interpolation scheme. The processed data from ENDF/B-VIII evaluated data showed good agreement with OpenMC provided JEFF-3.2 cross-section data. The value of multiplication factor at various cases intercomparison with two databases and compared with other codes showed satisfactory result, the variation of K_{inf} value was within 0.02% to 0.5% deviation from other codes. The findings of this study can be implemented in future works of nuclear fuel assembly or full core implementation of nuclear reactors. This work also implies the successful processing and conversion of ENDF/B-VIII nuclear data by implementing those in UO_2 and $UPuO_2$ fueled pincell.

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