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Examination and refinement of fine energy group structure for high temperature reactor analysis

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ABSTRACT

Multi-group energy structure SHEM-281 and -361 were refined using a Contributon and Point-Wise Cross Section Driven method (CPXSD). The Contributon and Point-Wise Cross Section Driven method was derived based on the product of the forward and adjoint angular fluxes, and the point-wise cross section of important isotope/material. It is an iterative method that selects effective fine- and broad-group energy structures for a problem of interest. The two selected criteria for determining fine energy group structure were 10 pcm relative deviation of $\Delta k/k$ for k-effective and 1% relative deviation for reaction rates. The energy group structure refinement was subdivided into fast, epithermal and thermal regions. Firstly, the refinement was done for fast region and a new library was created and applied in the fuel cell unit until the target criteria's are met. Similar procedure was repeated for epithermal and thermal regions. The dominant parameters for each region are considered as required, fission reaction rate for fast region, absorption reaction rate for epithermal region and absorption and fission reaction rates for thermal region.

1. Introduction

Fine energy group structures are of utmost importance for allowing accurate calculation of neutron group cross sections for reactor analysis. Neutron group cross sections are generated from continuous cross section data files that have been collected for the past decades by experimental measurements and theoretical calculations. These data files contain all of various types of neutron cross sections, e.g. scattering, absorption etc. for all the important nuclides resulting in a vast volume of data stored in standardized format in the Evaluated Nuclear Data File (ENDF-). ENDF/B data files are processed using NJOY through an object oriented Python Script named PyNjoy which is compatible to the Dragon code used for this work. NJOY is a nuclear data processing system that converts the evaluated nuclear data ENDF/B format into usable libraries for nuclear reactor analysis. It handles all nuclear reactor parameters such as resonances, Doppler broadening, heating, radiation damage, scattering, gas production, neutrons and charged particles, photo-atomic interactions, self-shielding, probability tables, photon production and high energy interactions. NJOY consists of a set of modules from which several can be selected to perform specific calculations. The objective of this work is to examine and refine the available energy group structures (SHEM-281 and -361) for high temperature reactors (HTR). They were previously developed and optimized for light water reactor (LWR) applications. The SHEM energy group structures addressed the fuel components as well as the structural materials expected to be present in LWR's (Hebert and Santamarina, 2008; Hfaiedh and Santamarina, 2005). It was verified to be accurate for both uranium and mixed oxide fuels in LWRs. Additionally, actinides were addressed extensively in that their resonant reactions are well covered by the structure. The uncertainty was whether the SHEM energy group structures are applicable to HTRs with graphite moderation and its high burnup applications without further modifications. Therefore it was necessary to examine this potential shortcoming of SHEM energy group structure, and be modified to cover all HTRs and deep burn related physical phenomena.

The HTR fuel designs, Pebble fuel element and Prismatic assembly lattice, were analyzed in this work. Pebble and cylindrical rods fuel elements are both embedded with tri-structural isotopic coated particles. These coated particles (CP) consists of a kernel (UO_2), low density carbon (buffer layer), pyrolytic carbon (inner and outer layers) and silicon carbide that serve as a radiation containment. This results in complex heterogeneous systems that occur between the particles in a graphite matrix, then between the fuel elements and other structural materials like moderator and a reflector (DeHart and Ulses, 2009). Thus there are significant changes in

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the physics of neutron slowing down, absorption and scattering processes in the HTRs compared to that which occur in the LWRs.

For example, neutron slowing down is governed by two processes, elastic and inelastic scattering where elastic scattering can easily occur with neutron of any energy while the inelastic scattering requires a sufficiently high energy to excite the target nucleus to a higher energy level. The slowing down process also depends on the atomic mass of a moderator, the lighter the nucleus the better the moderating ability. However, a moderator must exhibit low neutron absorption. Graphite (carbon) has the highest atomic mass, $M_C = 12$ of any moderator whereas the hydrogen in water has the lowest atomic mass $M_H = 1$. Therefore, during the slowing down of neutrons from the fast to thermal energies due to mainly elastic scattering, neutrons lose less energy per collision with graphite than hydrogen. It takes 118 collisions for neutrons to slow down to thermal energies in graphite whereas only 18 collisions are needed in hydrogen. The large energy changes that take place in LWRs allow the neutron to escape the resonances relatively often while slowing down in the epithermal energy region. It also allows the total energy spectrum to be divided into two broad energy groups, fast and thermal, for successful reactor analysis of the LWRs. This is not the case for graphite moderated HTRs, due to the extra number of scattering required for a neutron to slow down through the epithermal region, there is greater chance for the neutrons to be captured by the resonance cross sections. For this reason, more broad energy groups are required in analyzing HTRs.

2. Method

The refinement of the energy group structures were conducted using the Contributon and Point-Wise Cross Section Driven (CPXSD) method which was developed by Alpan and Haghighat, 2005. The CPXSD method was derived based on the product of the forward and adjoint angular fluxes, and the point-wise cross section of important isotope/material of interest (see Eq. (1)). It is an iterative method that selects effective fine- and broad-group structures for a problem of interest.

$$C(E) = \int_{v} dr \int_{4\pi} d\Omega \Psi(\vec{r}, E, \hat{\Omega}) \Psi^{+}(\vec{r}, E, \hat{\Omega}) \quad (1)$$

where $C(E)$ – is the energy dependent importance function, $\Psi(\vec{r}, E, \hat{\Omega})$, – is the angular flux and $\Psi^{+}(\vec{r}, E, \hat{\Omega})$ – is the adjoint flux dependent on position $\vec{r}$, energy (E) and direction $(\hat{\Omega})$. The fine energy group structure refinement followed in this work is as follows:

I. An initial multi-group energy structure was selected, SHEM-281 or -361 energy group structure.
II. Cross sections were generated for the initial multi-group energy structure using the established procedure of cross section generation relevant to DRAGON transport code.
III. The angular and adjoint flux calculations were performed to determine the importance function of the groups in the initial energy group structure of interest.
IV. After identifying the energy groups with higher importance, these energy groups were refined by the resonance structure of a spectrum representing the unit cell (fuel) by dividing the energy group into two or more energy groups.
V. When the refinement process was complete for all energy groups, the new energy group structure was used for cross section generation. The new cross section library was used to calculate the reaction rates and k-effective of the problem of interest.
VI. The reaction rates and k-effective calculated using the new library are compared with the results obtained from the previous library calculations. If the results are within a specified tolerance, the procedure ends; otherwise, the procedure is repeated.

3. Depletion analyses

Depletion analyses were conducted using the new refined energy group structure SHEM_TPN-531 (Ngeleka, 2012). Depletion is an important aspect of reactor analysis for the reactor safety and for the prediction of the economic performance of the reactor. It includes various nuclear reactions, and is described by the isotopic depletion rate equations where isotopic concentrations are solved as a function of time and position. Secondly, the multi-group transport/diffusion equations are solved for the neutron flux. The DRAGON code used for this work, use an EVO module (Marleau et al., 2010) wherein depletion equations for different isotopes in the library are solved using burnup chains as available in the generated library. The depletion analyses were performed at constant power in MW/tonne of initial uranium using burnup time steps (in Days), assuming linear flux/power changes. The burnup mixtures of the unit cell are solved using the rate equations describing the isotopic changes in the core composition during the reactor operation. The results are given in Section 5.

4. HTR materials

There are two forms of HTR's fuel used in this work. Pebble fuel element of 6 cm diameter and 5 cm fuel zone are used for Pebbled bed reactors. The latest design for Pebble fuel element has 15,000 CP's. Prismatic hexagonal blocks with 1.27 cm fuel channels diameter and 1.588 cm coolant channels are used for Prismatic reactors. Each cylinder in the hexagonal block has about 3000 CP's each. Both the Pebble and the cylindrical rod fuel elements are composed of TRISO coated particles (CP) that are embedded in a graphite matrix. The coated particle consists of a kernel of uranium dioxide (UO_2), buffer layer (low density carbon layer), inner pyrolytic carbon layer, silicon carbide layer and outer pyrolytic carbon layer. For detailed specifications of the fuel materials can be found in DeHart and Ulses (2009).

Table 1
Results for SHEM-281 and 407 energy group structures.

Group structure	Reaction rates	Energy range		
		Thermal	Epithermal	Fast
Pebble				
SHEM-281	Absorption (collisions/cm^3 s)	7.35093E−01	2.58643E−01	6.26975E−03
	Nu-fission (fissions/cm^3 s)	1.40377E+00	1.04519E−01	8.63650E−03
	k-Effective	1.51692 (convergence = 2.79E−09)		
SHEM_TPN-407	Absorption (collisions/cm^3 s)	7.35662E−01	2.58207E−01	6.13159E−03
	Nu-fission (fissions/cm^3 s)	1.40454E+00	1.03868E−01	8.48825E−03
	k-Effective	1.516901 (convergence = 9.15E−09)		