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Parameterized representation of macroscopic cross section in burn-up cycles

João Claudio B. Fiel *, Thiago F. Belo

Department of Nuclear Engineering, Military Institute of Engineering, Rio de Janeiro, Brazil

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ABSTRACT

Nuclear reactor core analysis involves neutronic modeling and the calculations require problem dependent nuclear data generated with few neutron energy groups, as for instance the neutron cross sections. The methods used to obtain these problem-dependent cross sections, in the reactor calculations, generally uses nuclear computer codes that require a large processing time and computational memory, making the process computationally very expensive. To provide the cross sections of rapidly and without the dependence of complex systems calculations, this work developed a set of parameterized macroscopic cross sections, based on the Tchebychev polynomials, by fitting the cross sections as a function of nuclear parameters, which include fuel temperature, moderator temperature and density. In this study is evaluated the problem-dependent about fission, scattering and capture cross sections for a typical PWR fuel element reactor, considering burn-up cycles. The analysis was carried out with the SCALE 6.1 code package. Tests realized as the temperature coefficient of reactivity, fast fission factor, and the comparison with direct calculations with the SCALE code system and with Lagrange polynomials show excellent agreements. The differences between the cross section parameterization methodology and the direct calculations based on the SCALE code system are less than 0.03%.

1. Introduction

The nuclear reactor design is based on control of several variables. These variables include the nature of the fuel and the moderator, core compositions and geometry, and removal of the heat which is generated mainly by fission and partly by radioactive decay. An essential part of the reactor design is the core specification, since this determines the neutron behavior in the system and hence the criticality conditions (Glasstone and Sesonske, 1994). Neutronic calculations are based on either transport or diffusion theory, which can be implemented by deterministic or stochastic method (Monte Carlo). In general the calculations require problem dependent nuclear data generated with few neutron energy groups, as for instance the neutron cross sections, which depend on the fuel element material composition as well as the thermal hydraulic parameters. During the reactor operation the fuel composition will change as fissile isotopes are consumed and fissions products are produced, resulting in a different behavior of the absorption cross section. These changes, in both space and time, which occur in the composition of the fuel, can be determinate by the fuel burn-up calculation.

Presently, analysis and studies of the macroscopic cross section, as a function of nuclear parameters, have shown very distinct behavior that cannot be represented by simply using linear interpolation. Indeed, a polynomial representation is more adequate for the data parameterization. Nevertheless, existing methods do not indicate explicitly the type of polynomial fit that best represents the problem-dependent cross section. The methods used to obtain these problem-dependent cross sections, in the reactor calculations, generally uses nuclear computer codes that require a large processing time and computational memory, making the process computationally very expensive. Therefore, new methods have been studied for the purpose of seeking alternative procedures to provide the cross sections of rapidly and safely without the dependence of complex systems calculations. Over the years, methods of few-groups cross section parameterization using mathematical processes such as stepwise regression (Zimin and Semenov, 2005), quasi-regression (Bokov, 2009) and sparse grids methods (Prinsloo et al., 2009), were elaborated and suggested.

It was developed (Fiel, 2013) a study of the cross section parameterization using Tchebychev polynomials based on problem dependent cross sections calculated with the SCALE code system for the zero cycle condition, i.e., the fresh PWR reactor. This

* Corresponding author.
E-mail addresses: fiel@ime.eb.br (J.C.B. Fiel), thiagofreitasbelo@gmail.com (T.F. Belo).

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methodology was used in this work to performing the analysis of homogenized macroscopic cross sections behavior in a PWR fuel element as a function of nuclear parameters, which include fuel temperature, moderator temperature and moderator density considering different burn-up cycles.

The purpose of this present work is complementing the preview analysis (Fiel, 2013) with a study of macroscopic cross section behavior considering burn-up cycles. In this study is evaluated the dependent problem about fission, scattering and capture cross sections. The results of the methodology presented in this paper are a set of parameterized cross sections based on the Tchebychev polynomials by fitting the cross sections as a function of these nuclear parameters. Tchebychev polynomials were chosen since they present some advantages when compared to other polynomials. Their parameterized function is the result of a method of minimizing error from a process that leads to better accuracy in the calculation of coefficients and in the estimate of polynomial fit at specific points. The cross sections parameterization can serve as an alternative for use in reactor calculations with few energy groups without the need to perform all the steps usually required for this type of calculation (Bjørn, 1981). Although the method developed in this work is suited for a particular type of fuel element of a typical PWR reactor it can be extended to any other PWR fuel element.

2. Methodology

Typical PWR fuel element (FE) with 12 integrated burnable absorber fuel rods was analyzed with the SCALE 6.1 code package, more specifically, the Monte Carlo code KENO-VI, the TRITON depletion sequence (T6-DEPL), and NEWT transport code (T-NEWT). The geometry and configuration of the FE was modeled with KENO-VI. The T6-DEPL sequence was used to perform the burn-up-dependent nuclide concentration determining the isotopic composition for the burn-up cycles. The problem-dependent macroscopic cross sections were generated by T-NEWT. The equations presented are functions of the following selected parameters: moderator temperature, fuel temperature and moderator density for a PWR FE (Leem et al., 2010). Dependent problem about fission, scattering and capture cross sections were obtained as a function of the selected parameters (Zimin and Semenov, 2005).

The 16×16 PWR FE modeled with the KENO code is displayed in Fig. 1. The FE has 236 rods, which 20 guide tubes and 12 burnable absorber rods. This FE has the specifications of a typical PWR FE (Westinghouse Pressurized Water Reactor Nuclear Power Plant, 1984), which isotopic compositions and geometrical configurations defined ANGRA II FSAR (ANGRA II, 1999). The first isotopic composition used in fresh reactor (zero cycle condition) was defined by four mixtures: UO_2 ($^{235}_{92}U$ enrichment 3 w/o), $^{10}_{5}B + H_2O$, $UO_2 + Gd_2O_3$ and Zircaloy. This composition was used as INPUT on the T6-DEPL three-dimensional (3-D), which was used to perform depletion calculations in the fuel rod and in the burnable absorber fuel rod. The T6-DEPL has the capability of simulating the depletion of multiple mixtures in a fuel assembly model, with allows a detailed representation of the local flux distribution for a specific fuel rod in the assembly to calculate fuel compositions. The depletion of the fuel and the burnable absorber fuel rod was simulated by T6-DEPL, using 36 MW/MTU of burn-up for all the bun-up cycles. The composition generated was consisted of 33 nuclides, 17 actinides and 16 fission products, which were important to fuel reactivity (i.e., nuclides with large neutron fission cross sections and nuclides with large neutron absorption cross sections). The 33 nuclides are the ones commonly considered in fuel compositions for burn-up credit criticality safety analyses that base validation of calculated nuclide concentrations on comparisons to available RCA (Radiochemical Assay) data (Radeluscu et al., 2014; Burnup Credit Criticality Safety Analyses, 2011).

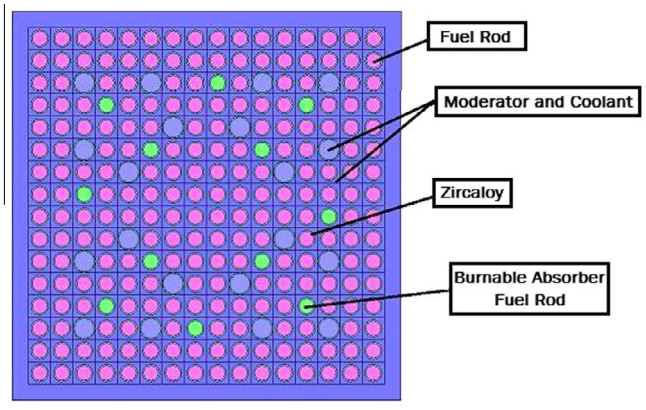

Fig. 1. Fuel element – top view.

The homogenized macroscopic cross sections were generated by T-NEWT using the isotopic compositions obtained in each cycle. T-NEWT calculations were performed using the SCALE 238-energy-group ENDF/B-VII library, named V7-238, which was developed based on the evaluated nuclear data libraries, ENDF/B-VII.0 (Chadwick et al., 2011). The results with the 238-energy groups were collapsed to two groups of energy. The ENDF/B-VII cross section data yield significantly more accurate calculated eigenvalues.

A careful study was performed to determine the set of independent parameters to be used in the parameterization. The homogenized macroscopic cross section performed by T-NEWT was generated as a function of only one variable, keeping the other variables fixed with reference values. The data ranges and the reference values used for the macroscopic cross sections generation are listed in Table 1. Tests utilizing projects parameters were carried out at the end of the process to verify the efficiency of the method. The calculations done with the SCALE 6.1 code served to benchmark the results obtained with the method based on the cross-section parameterization (Demaziére, 2009).

3. Cross section parameterization

The cross section parameterization was carried out based on the Tchebychev polynomials since they have some inherent advantages (Bokov et al., 2008) that are suited to our problem. These advantages of Tchebychev polynomials are:

- The first order roots of polynomials of can be used in polynomial interpolation.

Table 1
Analysis and reference values.

Nuclear parameters	Analysis values	Reference values
$^{235}_{92}U$ enrichment (w/0)	2; 2.5; 3; 4; 5	3
Boron concentration (ppm)	250; 500; 750; 850; 1000	500
Fuel temperature (K)	573; 673; 973; 1273; 1473	973
Moderator temperature (K)	300; 400; 500; 573; 613	573
Moderator density (g/cm^3)	1.003439; 0.945147; 0.842537; 0.727084; 0.617629	0.727084