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POLYNOMIAL PARAMETERIZED REPRESENTATION OF MACROSCOPIC CROSS SECTION FOR PWR REACTOR

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ABSTRACT

The purpose of this work is to describe, by means of Tchebychev polynomial, a parameterized representation of the homogenized macroscopic cross section for PWR fuel element as a function of soluble boron concentration, moderator temperature, fuel temperature, moderator density and $^{235}_{92}U$ enrichment. Analyzed cross sections are: fission, scattering, total, transport, absorption and capture. This parameterization enables a quick and easy determination of the problem-dependent cross-sections to be used in few groups calculations. The methodology presented here will enable to provide cross-sections values to perform PWR core calculations without the need to generate them based on computer code calculations using standard steps. The results obtained by parameterized cross-sections functions, when compared with the cross-section generated by SCALE code calculations, or when compared with k_{inf}, generated by MCNPX code calculations, show a difference of less than 0.7 percent.

1. INTRODUCTION

One of the most important and complex analysis of a nuclear reactor involves generating constant just appropriate groups, to determine the cross and diffusion coefficients for each core area. A wide variety of input data in computer programs is required for these calculations. The study of polynomial parameterization has been an alternative to improve this reality.

Nuclear reactor core analysis involves neutronic modeling, control of thermal hydraulic parameters and mechanical behavior of the fuel elements (Vyacheslav and Andrey, 2005).

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 on the thermal hydraulic parameters. These nuclear parameters are called state variables, which include fuel temperature, moderator temperature, moderator density, boron concentration and the fuel burn-up (Bokov, 2009). 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 aim of this work is to present a study of the cross-section parameterization using Chebyshev polynomials based on problem-dependent cross-sections calculated with the SCALE code (Bowman, 2011). Chebyshev 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 via a process that leads to better accuracy in the calculation of coefficients and in the estimation of the polynomial fit at specific points. To generate problem-dependent cross-sections the SCALE code system was used. It was used to analyze and to generate macroscopic cross sections for a fuel element (FE) of a typical PWR. The results of the methodology presented in this paper are a set of parameterized cross-sections based on the Chebyshev polynomials obtained by fitting the cross sections as a function of nuclear parameters. The new cross sections 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 calculations (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

The method for parameterization of the problem-dependent group cross-sections is based on cross-section generation using Monte Carlo calculations. The equations derived are functions of selected parameters, namely, ${}^{235}_{92}U$ enrichment, moderator temperature, boron concentration, fuel temperature and moderator density (Lee et al., 2010). The study was done for a PWR fuel element, which was modeled with the Monte Carlo code KENO of the SCALE system using the 238-group neutron structure. The Monte Carlo simulation was performed with 10,000 histories per generation. Problem dependent fission, total, scattering, capture, transport and absorption cross-sections were obtained as a function of the selected parameters (Zimin and Semenov, 2005). Tests were carried out at the end of the process to verify the efficiency of the method. The SCALE 238-group library, named V7-238, was developed based on the evaluated nuclear data libraries, ENDF/B-VII.0 (Chadwick et al., 2011). The analysis was divided in three steps, namely, determination of the problem dependent cross sections, parameterization and numerical validations.

2.1. Development

(a) In this section the methodology used in this work is presented. Prior to the cross section parameterization it were determined which parameters were to be used in the parameterization.

(b) The reference values for the five parameters are listed in Table 2.1.

Table 2.1 – Reference Values.

Nuclear Parameters	Reference Values
$^{235}_{92}U$ Enrichment	**3 $^{w}/_{0}$**
Boron Concentration	**500 ppm**
Fuel Temperature	**973 K**
Moderator Temperature	**573 K**
Moderator Density	**0.727084 g/cm^3**

The SCALE code version 6.1 was used to generate problem dependent cross-sections. In addition, the calculations done with the SCALE code served to benchmark the results obtained with the method based on the cross-section parameterization (Demaziére, 2009). The results with the 238-energy groups were collapsed to two groups of energy.

The isotopic composition of FE was defined by three mixtures, each one made up of UO_2, and $^{10}_{5}B$ + H_2O, Zircaloy.

For the cross-section generation it was used the reference values for the parameters as listed in Table 2.1. Figure 2.1 displays the PWR FE that was modeled with the KENO code:

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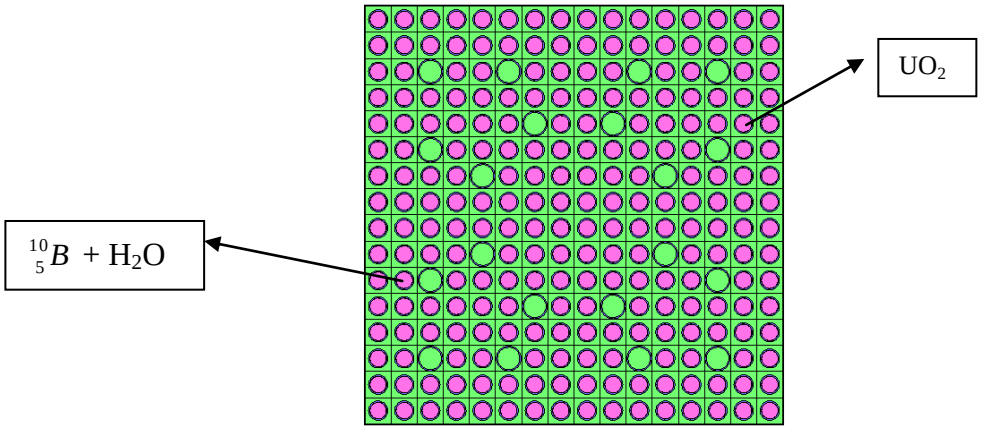

Figure 2.1 – Fuel Element – *Top View* (SCALE-KENO 3D)

2.1.1. Paramerization

The cross-section parameterization was carried out based on the Tchebychev polynomial since it presents some advantages (Bokov and Prinsloo, 2009) that are suited to our problem. These advantages of Tchebychev Polynomial are:

• They are important in approximation theory because the roots of polynomials of first order can be used in polynomial interpolation;

• They have the property of minimizing the error (standardizing it). The error is almost uniform for the entire range of analysis. Other polynomials also have these properties, but the Tchebychev ones are much more efficient. These deformities are present in other polynomials, better saying they present different errors within a range;

• The shape of Tchebychev polynomials is preferable since it leads to a general improved accuracy, and the calculation of the coefficients and estimating subsequent polynomial fit at specific points;

• They have the property of accelerating convergence on a recurring process.

In this section we present the determination of the Tchebychev coefficients after an analysis of the correlation coefficient value, which means that when the value is minimum, the polynomial reaches the maximum fitting of the curve.

In the process of searching for the polynomial description we wish to approximate the set of data points as closely as possible with a specified function (Chebyshev polynomial), which is as smooth as possible. The smoothness requirement is met by limiting the number of coefficients allowed in the fitting function, for example, by restricting the polynomial degree as in the case of Chebyshev polynomials. Given a particular number of coefficients in the function in question, the fitting routines, like E01AEF from the Numerical Algorithmic Group (NAG) library (Huddleston, 1974), determine the value of the coefficients such that the distance of the function from the data points is as small as a possible. The user decides the necessary balance by comparing a selection of such fits having different numbers of coefficients. If the number of coefficients is too low, the approximation to the data will be poor. If the number is too high, the fit will be too close to the data, essentially following the random errors and tending to have unwanted fluctuations between the data points. A measure of the distance between the set of data points and fitting function f(y) is needed. The distance from a single data point (x, y) to the function can simply be taken as er = yr _ f(xr), and is called the residual of the point. After the determination of the coefficients, the Chebyshev polynomials associated to each type of cross sections were written, for the fast and thermal energy groups. For each set of polynomials there was a variation of only one nuclear parameter while the other parameters was kept fixed with the reference values.

Throughout this paper, f(y) means the cross section written as a function of a nuclear parameter as listed in Table 2.1 for the fast and thermal energy group. A set of polynomials functions for each type of cross-section is constructed and the polynomials are written as follows:

$$f(y,) = a_0 T_0(y) + a_1 T_1(y) + a_2 T_2(y) + ... + a_n T_n(y), \quad (1)$$

where a_i is the Tchebychev coefficient, $T_i\ (y)$ is the polynomial of the first kind with Tchebychev argument y, with $T_0\ (y) = 1$; $T_1\ (y) = y$; $T_2\ (y) = 2y^2 - 1$; $T_3\ (y) = 4y^3 - 3y$; $T_4\ (y) = 8y^4 - 8y^2 + 1$; etc… and y varies in the range of –1 to +1 according to the expression:

$$y = \frac{2Y - Y_{\min} - Y_{\max}}{Y_{\max} - Y_{\min}}, \quad (2)$$

where Y is the value of the variable under study (nuclear parameter), Y_{max} and Y_{min} define the maximum and minimum values of Y among the analysis interval.

For a point chosen within the analysis interval of any nuclear parameter considered, the values of the cross section were obtained with the polynomial functions. Then, the cross sections obtained directly with the SCALE system were compared with the results obtained by polynomial functions. In general the agreement between the polynomial interpolation and the SCALE calculations were very good.

3. CROSS-SECTION PARAMETERIZATION

The cross section representation for each parameter listed in Table 2.1 is presented. Tables below show the parameterized polynomials functions for the analyzed cross-section as a function of state variables. In these tables *f(y)* means cross section, y means argument and Y means nuclear parameter like fuel temperature, moderator temperature, moderator density, enrichment and concentrate boron, where $y = \frac{2Y - Y_{\min} - Y_{\max}}{Y_{\max} - Y_{\min}}$.

3.1 - Cross Section as a Function of Fuel Temperature (T_F)

After the determination of the Chebyshev coefficients the parameterized polynomials were written as a function of the fuel temperature considering a variation of only one variable and keeping the remaining variables fixed of the reference values. The values of fuel temperature (in unit of Kelvin) used in this study to generate the cross sections were in the interval of 573–1473 K. The behavior of the macroscopic cross sections represented by polynomial expansions is described in Table 3.1. It can be observed that an increase in the fuel temperature leads to an increase of the resonant captures due to the Doppler broadening effect and consequently leading to an increase in the resonance absorption. The fission cross-section for the fast group is not very sensitive to the variation in fuel temperature and is practically constant whereas for the thermal energy region the fission cross-section decreases with increasing temperature.

Table 3.1 – Cross-section as a function of the fuel temperature

Cross Section	Group	Polynomials
Fission	Fast	0.0022840
	Thermal	$0.0422080 - 0.0002000y$
Total	Fast	$0.5268330 + 0.0003500y$
	Thermal	$1.2372350 - 0.0006160y - 0.0000001y^3$
Scattering	Fast	$0.5179500 + 0.0001500y$
	Thermal	$1.1704739 - 0.0003000y - 0.0001666y + 0.0001333y^3$
Absorption	Fast	$0.0089340 + 0.0002500y$
	Thermal	$0.0666890 - 0.0002500y$
Capture	Fast	$0.0067250 + 0.0002500y$
	Thermal	$0.0244810 - 0.0000500y$
Nu-Fission	Fast	0.0056980
	Thermal	$0.1028510 - 0.0004670y + 0.0001000y^2$
Transport	Fast	$0.2140080 + 0.0002160y + 0.0000490y^2 - 0.0003330y^3$
	Thermal	$0.74801400 - 0.0004500y$
Scattering 1-1	_____	$0.498700 + 0.0003000y$
Scattering 1-2	_____	$0.0192500 - 0.0002000y$
Scattering 2-2	_____	$1.1704739 - 0.0003000y - 0.0001666y^2 + 0.0001333y^3$

3.2 Cross-section as a function of the moderator (T_M).

The parameterized cross sections were obtained as a function of the moderator temperature, considering the variation of only one parameter while the other variables were kept fixed with the reference values. In this study, Y means moderator temperature which values are in the interval 300–613 K, with Y_{max} = 613 K and Y_{min} = 300 K. Table 3.2 presents the parameterized polynomials for the analyzed cross sections as a function of the moderator temperature. It can be seen from Table 3.2 that the macroscopic cross sections represented by the polynomial expansion increase with the moderator temperature leading to an increase in resonance absorption so that there is an increase in the absorption rate and consequently leading to a decrease in the number of fissions in the nuclear fuel. As the moderator temperature rises, keeping the density constant, there is a hardening of the neutron spectrum, which in turn results in an increase of the ‘‘low-lying’’ resonance absorption. These effects lead to a more negative coefficient of reactivity.

Table 3.2 – Cross-Section as function of the moderator temperature

Cross Section	Group	Polynomials
Fission	Fast	0.0022834
	Thermal	$0.0417122 - 0.0017278y + 0.0028334y^2 - 0.0016000y^3$
Total	Fast	$0.5267833 + 0.0000500y;$
	Thermal	$1.2358101-0.0096648y+ 0.0341739y^2 - 0.0309777y^3$
Scattering	Fast	$0.517925 + 0.0000500y$
	Thermal	$1.1822578-0.0074759y+ 0.0064236y^2 - 0.0293695y^3$
Absorption	Fast	0.0089084
	Thermal	$0.0663955 - 0.0025278y + 0.0044000y^2 - 0.0027333y^3$
Capture	Fast	0.0067250
	Thermal	$0.0243334 - 0.0007667y + 0.0016666y^2 - 0.0014000y^3$
Nu-Fission	Fast	0.0056973
	Thermal	$0.1023001-0.0040223y+ 0.0070223y^2 - 0.0041333y^3$
Transport	Fast	0.2140277
	Thermal	$0.7475240 - 0.0062425y + 0.0107739y^2 - 0.006711y^3$
Scattering 1-1	_____	$0.4986500 + 0.0000500y$
Scattering 1-2	_____	0.0192500
Scattering 2-2	_____	$1.1822578-0.0074759y+ 0.0064236y^2 - 0.0293695y^3$

3.3 – Cross-section as a function of the moderator density (d_M)

In this section the parameterized polynomial representation of the cross-section is presented as a function of the moderator density (in g/cm3), considering a variation of only one variable while the other variables were kept constant with the values of reference. The moderator density values used in the cross-section generation are from 0.617629 to 1.003439 g/cm3, where Ymax = 1.003439 and Ymin = 0.617629 g/cm3. Table 3.3 presents the parameterized polynomials for the analyzed cross-section as a function of the moderator density. Figs. 3.1–3.4 display the behavior of the fast and thermal group cross sections as a function of the moderator density. Fig. 3.1 shows the behavior of the transport, scattering 1–1, total and scattering fast group cross sections. Fig. 3.1 shows the behavior of the fission, scattering 1–2, absorption, capture and nu-fission fast group cross sections. Fig. 3.3 shows the behavior of the fission, absorption, capture and nu-fission thermal group cross sections and Fig. 3.4 shows the behavior of the total, scattering and transport fast group cross sections.

Table 3.3 – Cross-section as a function of the moderator density

Cross Section	Group	Polynomials
Fission	Fast	$0.0022084 - 0{,}0000500y$
	Thermal	$0.0369483 - 0.0032167y + 0.0108000y^2 + 0.0011334y^3$
Total	Fast	$0.5124083 - 0.1417500y + 0.0562000y^2 + 0.0488000y^3$
	Thermal	$1.2755675 - 0.4846100y + 0.0189223y^2 + 0.1630667y^3$
Scattering	Fast	$0.5036000 + 0.0683500y + 0.0560000y^2 + 0.0486000y^3$
	Thermal	$1.123121 - 0.1546394y + 0.1895223y^2 + 0.1597333y^3$
Absorption	Fast	$0.0088834 - 0.0005000y + 0.0001000y^2 + 0.0002000y^3$
	Thermal	$0.7129538 - 0.0087500y + 0.0030000y^2 + 0.0031334y^3$
Capture	Fast	$0.0066750 - 0.0004000y + 0.0001000y^2 + 0.0002000y^3$
	Thermal	$0.0239556 - 0.0055334y + 0.0021000y^2 + 0.0020000y^3$
Nu-Fission	Fast	$0.0056723 - 0.0003500y + 0.001000y^2 + 0.0002000y^3$
	Thermal	$0.1021631 - 0.0076963y + 0.0022333y^2 + 0.0025925y^3$
Transport	Fast	$0.2105916 - 0.0340500y + 0.0013500y^2 + 0.0118000y^3$
	Thermal	$0.7205397 - 0.2701499y + 0.1102666y^2 + 0.0920000y^3$
Scattering 1-1	_____	$0.4852000 - 0.1325500y + 0.0526000y^2 + 0.0456000y^3$
Scattering 1-2	_____	$0.0183750 - 0.0087500y + 0.0035000y^2 + 0.0030000y^3$
Scattering 2-2	_____	$1.1231210 - 0.1546394y + 0.1895223y^2 + 0.1597333y^3$

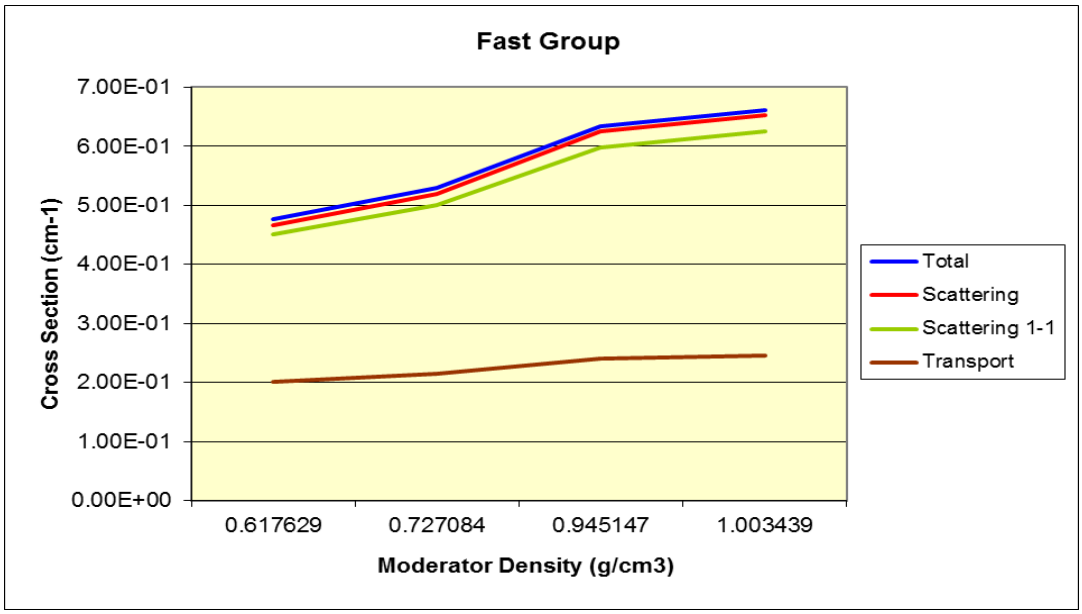

Fig 3.1 - Behavior of the Total, Scattering 1-1, Transport and Scattering of the fast group cross sections in function of moderator density

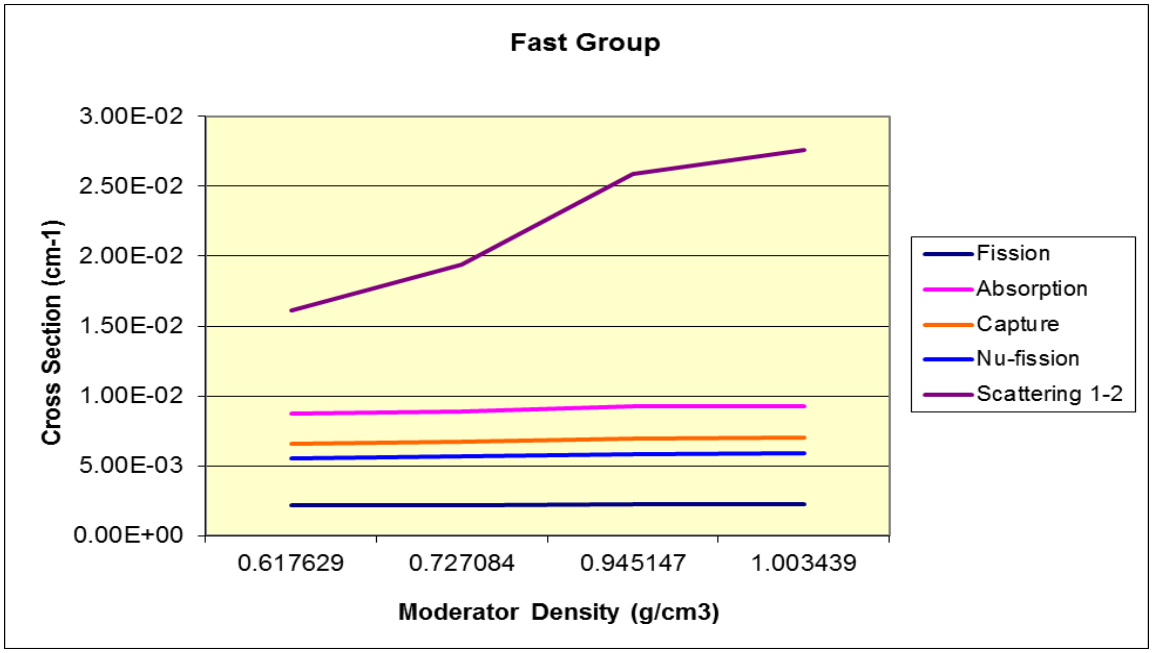

Fig 3.2 - Behavior of the Fission, Absorption, Capture, Nu-Fission and Scattering 1-2 fast group cross sections in function of moderator density

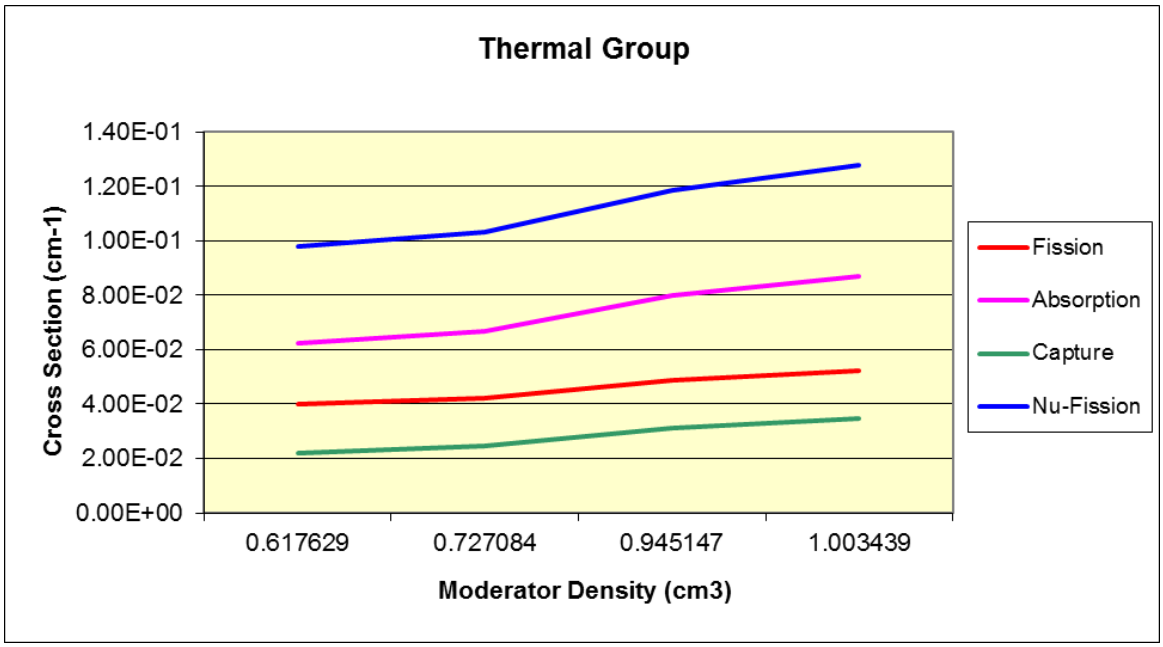

Fig 3.3 - Behaviour of the Fission, Absorption, Capture and Nu-Fission thermal group cross sections in function of moderator density

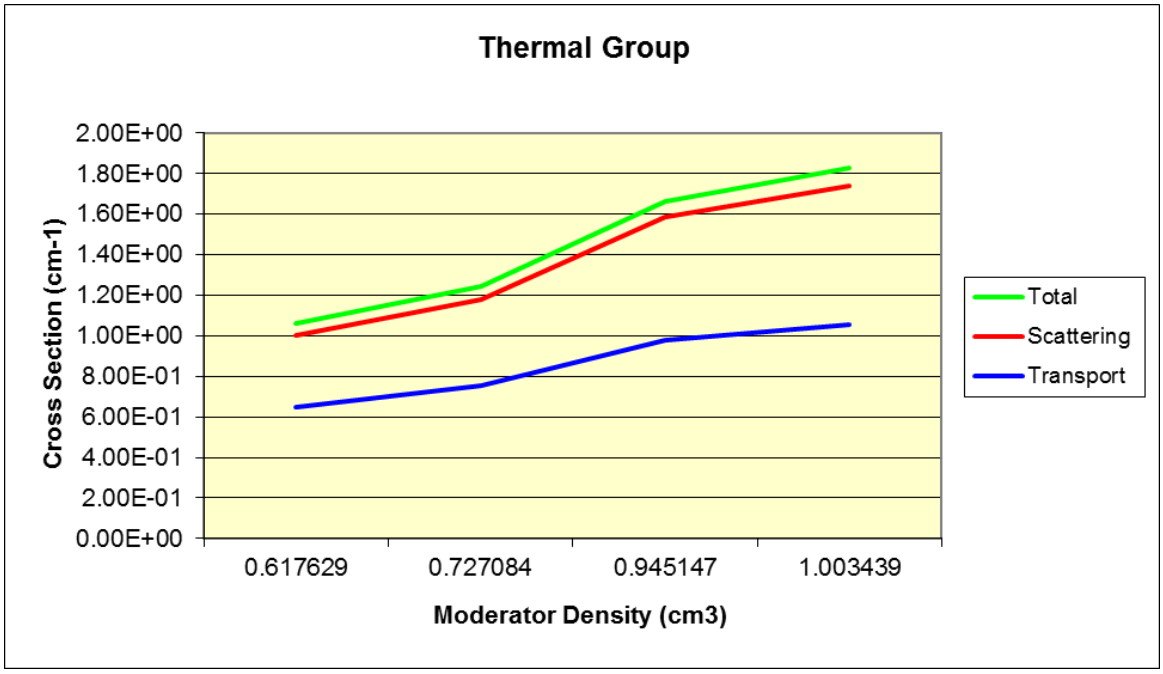

Fig 3.4 - Behavior of the Total, Scattering and Transport thermal group cross sections in function of moderator density

3.4 – Cross-section in function of the boron concentration (C_B).

The cross-section parameterization was done as a function of soluble boron concentration considering a variation of only one variable while keeping the remaining variables fixed with the reference values. The values of boron concentration (in ppm) used in the study to generate cross-sections were 250, 500, 750, and 1000 ppm, respectively, within the analysis interval of 250–1000 ppm. Table 3.4 presents the analyzed cross section as a function of the boron concentration. In this table f(y) means cross section, y means argument and Y means boron concentration, with Y_{max} = 1000 and Y_{min} = 250 ppm. The polynomial expansions given in Table 3.4, described in terms of the boron concentrations, show an increase in absorption and therefore a reduction in the number of fissions with an increase of the boron concentration. Due to the boric acid (H_3BO_3) high neutron capture cross-section (20% of 10B in natural boron) the absorption of neutrons leads to a decrease in the multiplication factor.

Table 3.4 – Cross-section in function of the boron concentration (C_B)

Cross Section	Group	Polynomials
Fission	Fast	0.0021840
	Thermal	$0.0418750 + 0.0000830y + 0.0002000y^2 - 0.0006000y^3$
Total	Fast	$0.5268080 - 0.0000008y$
	Thermal	$1.2376869 - 0.0001500y + 0.0013666y^2 - 0.0040666y^3$
Scattering	Fast	0.5179500
	Thermal	$1.1662150 + 0.0004780y + 0.0023330y^2 - 0.0068000y^3$
Absorption	Fast	$0.0089340 + 0.0000500y$
	Thermal	$0.0683640 - 0.0001830y - 0.0008000y^2 + 0.0027330y^3$
Capture	Fast	$0.0067250 + 0.0000500y$
	Thermal	$0.0264680 - 0.0001760y - 0{,}0010000y^2 + 0.0033120y^3$
Nu-Fission	Fast	0.0056980
	Thermal	$0.1020680 + 0.0000170y + 0.0005000y^2 - 0.0012670y^3$
Transport	Fast	0.2140660
	Thermal	$0.7453200 + 0.0012610y + 0.0015330y^2 - 0.0044000y^3$
Scattering 1-1	_____	0.4987000
Scattering 1-2	_____	0.0192500
Scattering 2-2	_____	$1.1662150 + 0.0004780y + 0.0023330y^2 - 0.0068000y^3$

3.5 – Cross-section as a function of the $^{235}_{92}U$ enrichment (E)

The parameterization of the cross section is presented as a function of $^{235}_{92}U$ enrichment considering a variation of only one variable while the other variables were kept fixed with the reference values. The values of the $^{235}_{92}U$ enrichment used in the study were 2, 3, 4, 5 $^{W}/_{0}$, respectively. Table 3.5 presents the parameterized polynomials for the analyzed cross section as a function of the $^{235}_{92}U$ enrichment. In this analysis $Y_{max} = 5\ ^{W}/_{0}$ and $Y_{min} = 2\ ^{W}/_{0}$.

Table 3.5 – Cross Section as a function of the $^{235}_{92}U$ Enrichment (E)

Cross Section	Group	Polynomials
Fission	Fast	0.0021840
	Thermal	$0.0418750 + 0.0000830y + 0.0002000y^2 - 0.0006000y^3$
Total	Fast	$0.5268080 - 0.0000008y$
	Thermal	$1.2376869 - 0.0001500y + 0.0013666y^2 - 0.0040666y^3$
Scattering	Fast	0.5179500
	Thermal	$1.1662150 + 0.0004780y + 0.0023330y^2 - 0.0068000y^3$
Absorption	Fast	$0.0089340 + 0.000050y$
	Thermal	$0.0683640 - 0.0001830y - 0.0008000y^2 + 0.0027330y^3$
Capture	Fast	$0.0067250 + 0.0000500y$
	Thermal	$0.0264680 - 0.0001760y - 0.0010000y^2 + 0.0033120y^3$
Nu-Sigf	Fast	0.0056980
	Thermal	$0.1020680 + 0.0000170y + 0.0005000y^2 - 0.0012670y^3$
Transport	Fast	0.2140660
	Thermal	$0.7453200 + 0.0012610y + 0.0015330y^2 - 0.0044000y^3$
Scattering 1-1	_____	0.4987000
Scattering 1-2	_____	0.0192500
Scattering 2-2	_____	$1.1662150 + 0.0004780y + 0.0023330y^2 - 0.0068000y^3$

4. NUMERICAL VALIDATION

The efficiency of the method developed based on the crosssection parameterization is tested against results obtained with direct calculations using the SCALE code system. The temperature coefficient of reactivity (q(T)) calculated using results from the methods developed and the results from the SCALE code system.

4.1 – Comparison of Results between SCALE and Developed Method

As an example, the moderator temperature value of 456.5 K was chosen to compare the results of SCALE calculations and results based on the cross-section parameterization. The remaining variables were kept with the reference values. Two energy-groups cross section, namely, fission, total, scattering, transport, To check the accuracy and efficiency between Tchebychev and polynomial fitting, we compared the associated errors at each adjusted points for each fitting functions. We observe that the Tchebychev polynomial advantages over the others are:

1 – The first order root can be used in polynomial interpolation;

2 –Minimizing the error (standardizing it);

3 - Accelerating convergence.

Table 4.1 – Comparison of Results between SCALE and Developed Method

Cross Section	Group	Tchebychev Polynomials	Interpolation	SCALE	Deviation
Fission	Fast	$0,002283$	0,00228	0,00228	0,0040%
	Thermal	$0,041712 - 0,001728y + 0,002833y^2 - 0,001600y^3$	0,04171	0,04158	0,3199%
Total	Fast	$0,526783 + 0,000050y$	0,52678	0,52576	0,1940%
	Thermal	$1,235810 - 0,009665y + 0,034174y^2 - 0,030978y^3$	1,23581	1,26356	0,6000%
Scattering	Fast	$0,517925 + 0,000050y$	0,51793	0,51788	0,0001%
	Thermal	$1,182258 - 0,007476y + 0,006424y^2 - 0,029370y^3$	1,18226	1,18321	0,0803%
Absorption	Fast	$0,0089084$	0,00891	0,00892	0,1121%
	Thermal	$0,066396 - 0,002528y + 0,004400y^2 - 0,002733y^3$	0,06640	0,07034	0,3940%
Capture	Fast	$0,006725$	0,00673	0,00670	0,4478%
	Thermal	$0,024333 - 0,000767y + 0,001667y^2 - 0,001400y^3$	0,02433	0,02442	0,3685%
Nu-Fission	Fast	$0,005697$	0,00570	0,00569	0,1757%
	Thermal	$0,102300 - 0,004022y + 0,007022y^2 - 0,004133y^3$	0,10230	0,10302	0,6989%
Transport	Fast	$0,214028$	0,21403	0,21404	0,0047%
	Thermal	$0,747524 - 0,006243y + 0,010774^2 - 0,006711y^3$	0,74752	0,75715	0,0127%
Scattering 1-1	_____	$0,49865 + 0,00005y$	0,49865	0.49863	0,0034%
Scattering 1-2	_____	$0,019250$	0,01925	0,01925	0,0067%
Scattering 2-2	_____	$1,182258 - 0,007476y + 0,006424y^2 - 0,029370y^3$	1,18226	1,18321	0,0803%

4.2 – Comparison of temperature coefficients of reactivity calculated using the results from developed method (Tchebychev Polynomials) and using results from the SCALE system

From the standpoint of reactor safety and control there is no parameter of importance than the temperature coefficient of reactivity. We have used the temperature coefficient of reactivity to test the accuracy of the cross-sections parameterized methodology. Tables 4.2 and 4.3 display a comparison between k_1 values for the temperatures T_2 = 600 and T_1 = 590 K calculated with the SCALE code system and by the cross-sections parameterization methodology. The percentage difference between the two calculations is very small which indicates that the cross-section parameterization methodology reproduces very well the direct calculations using the SCALE code system. In Table 4.3, we can see a good approximation of the results. In this work q(T) is expressed in Dk/k.

Table 4.2 – Comparison between Tchebychev Polynomials and SCALE system

Results	$k_{\inf}(T_2)$	$k_{\inf}(T_1)$
SCALE	0,93206701 ± 0,00015	0,93409561 ± 0,00029
Tchebychev Polynomials	0,932384	0,9344781
Deviation	0,03401%	0,04094%

In table 4.3, we can see a good approximation of the results. In this work $\rho(T)$ is expressed in Δk/k.

Table 4.3 – Comparison between cross-sections parameterized and SCALE system

Results	$\rho(T_2)$	$\rho(T_1)$	α_T
SCALE	-0,0728842 Δk/k	-0,0701160 Δk/k	-0,0002768
Tchebychev Polynomials	-0,0725194 Δk/k	-0,0705542 Δk/k	-0,0001965
Deviation	0,07075%	0,0438%	_____

4. CONCLUSIONS

The work presented in this paper describes a methodology for the parameterization of problem-dependent cross-sections as a function of reactor parameters. The method is offered as an alternative to cross-section determination using few energy groups in
PWR fuel element calculations. Another important advantage of the cross-section parameterization methodology is that once the cross-section data have been parameterized they can be stored and easily used in very simple computer devices for fast calculations.
The results of comparison with direct calculations with the SCALE code system show excellent agreements. Although the methodology has been derived for a particular reactor configuration the method can be easily extended for other reactor configurations. It is suggested that the methodology presented here can also be extended to include reactor burnup.

REFERENCES

ANDREAS Fessier, DONALD L. Smith, 2002, Parameter sensitivities in nuclear reaction cross-section calculations, Annals of Nuclear Energy;
Bjørn Thorlaksen, Construction Of Pwr Nuclear Cross Sections For Transient Calculations. Test of the Anti-Program against Two dim, Risø National Laboratory, DK 4000 Roskilde, Denmark, May 1981.
BOKOV, P.M., Prinsloo, R.H., Tomašević, D.I., Reitsma, F., 2008. A quasi-regression method for automated cross-section parameterization: PBMR benchmark example. In: PHYSOR'2008 – International Conference on Reactor Physics, Nuclear Power: A

Sustainable Resource, Interlaken, Switzerland, September 14–19, 2008;
DEMAZIÉRE, C.2009, Development of computational methods and their applications for analysis of nuclear power plants, International Journal of Nuclear Energy Science and Technology 4 (4), 287-298.
DUDERSTADT, JAMES J., HAMILTON, LOUIS J. Nuclear Reactor Analysis, John Wiley & Sons, Inc. (1976).
JAN DUFEK, Building the nodal nuclear data dependences in a many-dimensional state-variable space, Annals of Nuclear Energy Vol. 38, issue 7, July 2011, pg. 1569-1537;
MARTINEZ**,** A. S. ; ROSA, L. P. . Análise da Moderação de Nêutrons Considerando o Espalhamento Linearmente Anisótropico no Centro de Massa. Revista Brasileira de Física, Brasil, v. 8, n.3, p. 536-549, 1978;

M.-J. LEE, J. G. Joo, D. Lee, and K. Smith, "Multigroup Monte Carlo Reactor Calculation with Coarse Mesh Finite Difference Formulation for Real Variance Reduction," *Proc. Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2010 (SNA + MC2010)*, Tokyo, Japan, October 17-21, 2010.

M. ABRAMOWITZ, I.A. Stegun, Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables, (Ninth Dover Printing, Tenth GPO Printing Edition) Dover, New York (1964);

PAVEL, M. Bokov, Automated few-group cross-section parameterization based on quasi-regression, Annals of Nuclear Energy 36 (2009) 1215-1223;
VYACHESLAV G. Zimin, ANDREY A. Semenov, Building neutron cross section dependencies for few-group reactor calculations using stepwise regression, Annals of Nuclear Energy Vol. 32, issue 1, January 2005, pg. 119-136;
V.G. ZIMIN, A.A. SEMENOV, Building neutron cross-section dependencies for few-group reactor calculations using step-wise regression, Annals of Nuclear Energy, 32 (2005), pp. 119–136;
ENDF/B-VII.1 Nuclear Data for Science and Technology: Cross Sections, Covariances, Fission Product Yields and Decay Data, M.B. Chadwick, et. al., Nuclear Data Sheets Volume 112, Issue 12, December 2011, Pages 2887–2996

JEFF-3.1 NEA/OECD; "The JEFF-3.1 project: Complete content of the JEFF- 3.1 evaluated nuclear data library", June 2, 2005, NEA#0607

JENDL-4.0: A New Library for Nuclear Science and Engineering, K. Shibata, O. Iwamoto, T. Nakagawa, N. Iwamoto, A. Ichihara, S. Kunieda, S. Chiba, K. Furutaka, N. Otuka, T. Ohsawa, T. Murata, H. Matsunobu, A. Zukeran, S. Kamada, and J. Katakura: J. Nucl. Sci. Technol. 48(1), 1-30 (2011)

CHIHARA, T.S., An Introduction to Orthogonal Polynomials, Mathematics and its Applications Series, Gordonand Breach, New York, 1978.

RIVLIN, T.J., Chebyshev Polynomials, John Wiley & Sons Inc., New York, 1990.
SPIEGEL, Murray Ralph, Schaum's outline series Mathematical of Formulas and Tables; McGraw-Hill,Inc., 1968.
CLENSHAW, C. W. A Note on the Summation of Chebyshev Series. MTAC, 9, pp. 118-120, 1955.

HUDDLESTON, R.E., CDC 6600 routines for the interpolation of data and of data with derivatives. Sandia Laboratories. Reprint SLL-74-0214, 1974.
KROGH, F.T., Efficient algorithms for polynomial interpolation and numerical differentiation. Math. Comp., 24, pp. 185-190, 1970.
COX, M. G. A Data-Fitting Package for the Non-Specialist User. Report NAC40, National Physical Laboratory, Teddington, Middlesex, 1973.
COX, M. G. and Hayes, J.G. Curve Fitting: a Guide and Suite of Algorithms for the Non-Specialist User. Report NAC26, National Physical Laboratory, Teddington, Middlesex, 1973.
GENTLEMAN, W.M. An Error Analysis of Goertzel's (Watt's), Method for Computing Fourrier Coefficients. Comp. J., 12, pp. 160-165, 1969.
CLENSHAW, C.W. and HAYES, J.G. Curve and Surface Fitting. J. Inst. Maths. Applics., 1, 1965, pp. 164-183.
HAYES, J. G. Curve fitting by polynomials in one variable. Numerical Approximation to Functions and Data, edited by J. G. Hayes. The Athlone Press, 1970, Chapter 5.