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Building neutron cross-section dependencies for few-group reactor calculations using stepwise regression

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Abstract

Approximation of few-group neutron cross-sections by functions of burnup and thermal-hydraulics parameters of a fuel cell is considered. The cross-section is written as a sum of two terms: the base cross-section, which depends only on burnup and is computed under the nominal reactor core conditions, and the deviation, which depends on burnup and thermal-hydraulics variables of the cell. A one-dimensional dependence of the base cross-section is interpolated by a cubic spline. Multi-dimensional dependencies of the deviation are approximated by a polynomial. Construction of the polynomial is performed by a best-fitting selection of the polynomial terms using the stepwise regression algorithm. The number of terms to satisfy a user-given accuracy of approximation is minimized.

As an example, approximation of a set of two-group macro and micro cross-sections as functions of burnup, coolant and fuel temperature, coolant density and boron concentration is considered for a fuel pin cell of a VVER reactor. The constructed five-dimensional polynomial approximating cross-sections within 0.05% tolerance has about 20 terms for fast group cross-sections and 50 terms for thermal group cross-sections. The error of approximation is verified on the two data sets: the initial data used for approximation and the test data being computed on randomly selected points. Mean square and maximum errors are comparable for

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all the cross-sections for both sets of data. These results show that the initial data can be applied to control the approximation error.

1. Introduction

Nuclear reactor neutron calculations require few-group neutron cross-sections, which depend on the material composition of a cell or fuel assembly (FA) and on thermal-hydraulics parameters. These characteristics of the cell are called state variables. For example, the state variables of a VVER cell include fuel burnup, fuel and coolant temperatures, coolant density and boron concentration. To build the dependencies of neutron cross-sections on the state variables, the variable domain is covered by a mesh and the cross-sections are computed at the mesh points. The calculations are usually organized as follows. Burnup calculation of FA is performed under the nominal constant values of the state variables. This is called the base calculation. Additional branch calculations are executed at each time step of the burnup calculation to describe cross-section dependencies on the cell state variables. Then, a computed set of the neutron cross-sections is interpolated or approximated over the entire variable domain.

In this paper, the two problems associated with the neutron cross-section preparation are considered:

- building a mesh used in the neutron cross-section calculations;
- selecting a procedure for approximation of the neutron cross-section dependencies.

Let us consider traditional approaches to treat these problems. A regular Cartesian mesh is often applied to compute the neutron cross-sections. The regular mesh has about 2000 mesh points for PWR FA resulting in considerable time being needed to perform the neutron cross-section calculations even on modern workstations (Smith, 2000).

Multi-dimensional table interpolation or *approximation by a function of several variables* are normally applied to approximate cross-section over a variable domain. For example, five-dimensional linear table interpolation is used to describe the neutron cross-section dependencies of VVER FA (Semenov et al., 1998), while neutron cross-sections of RBMK channels are approximated by a three-dimensional polynomial (Turski et al., 1997). Both approaches have their advantages and disadvantages.

In the case of table interpolation, the cross-sections are computed by the linear or cubic interpolation of values at the mesh points. For a fixed order of interpolation accuracy can be increased by refining the mesh. The main advantage of this approach that it is very general, i.e. an interpolation algorithm does not depend on a functional form of interpolated data. The most serious disadvantages are low accuracy of linear interpolation and a requirement to use a regular Cartesian mesh for the cross-section calculations. As a result, the required number of the mesh points is

considerable, resulting, first in several thousands FA calculations to generate the neutron cross-sections and, second, in a large neutron cross-section library. For example, Smith (2000) reported that about 2000 mesh points are needed to generate the neutron cross-section dependencies of a PWR FA. That results in 1 Mb of neutron cross-section data for one FA and about 100 Mb of neutron cross-section library for a typical PWR core (Smith, 2000). A large neutron cross-section library results not only in the considerable memory requirement, but also increases the computing time of the interpolation procedure due to an increase in the time needed for data access. The low accuracy of linear interpolation is clearly demonstrated in the case of reactivity effect calculations, where not only the accuracy of the neutron cross-section representation is important, but also the accuracy of the approximation of neutron cross-section derivatives is significant.

Approximation of cross-sections by functions of several variables also has certain advantages. First of all, application of a regular Cartesian mesh is not necessary in this case. An arbitrary mesh can be applied offering the potential to decrease the number of the mesh points and the associated computing time of FA calculations. Second, as a result of approximation, an initial data set having at least hundreds of data points is reduced to tens of polynomial coefficients. Thus, the size of the neutron cross-section library is reduced by an order of magnitude in a comparison with the table interpolation. The main problem associated with the application of the approximation procedure is selection of a polynomial form, which is usually performed "by trial and error as providing the best compromise between the needs for accuracy on the one hand and simplicity on the other" (Turski et al., 1997).

In this paper, we suggest solutions for both the mesh selection and approximation procedure. A mesh for neutron cross-section calculations is constructed as a combination of the one-dimensional regular mesh for burnup and the uniformly distributed mesh for branch calculations, generated using quasi-random sequences of Sobol'. These topics are considered in Section 2. A combined interpolation/approximation procedure to generate neutron cross-section dependencies is given in Section 3. A neutron cross-section is represented as a sum of two terms: the base cross-section, which depends only on burnup and the deviation, which depends on all the FA state variables. The one-dimensional dependence of the base cross-section on burnup is interpolated by a cubic spline. The dependencies of the deviation are approximated by a multi-dimensional polynomial. The main feature of the presented approach is an automatic selection of the optimal polynomial form, which satisfies a user-given accuracy of approximation. Optimality is considered in the sense of the minimum number of polynomial terms for the given accuracy. Construction of an optimal polynomial is performed by best-fitting subset selection using the stepwise regression algorithm. Basic concepts of regression analysis are given in Section 3.1. Tests of significance of the constructed regression model and the individual regression coefficients are presented in Section 3.2. Section 3.3 describes the stepwise regression algorithm applied to construct the optimal approximating polynomial. In Section 4, approximation of a set of two-group macro and micro cross-sections of a VVER fuel pin cell by functions of burnup, coolant and fuel temperature, coolant density and boron concentration is considered. Conclusions are given in Section 5.

2. Building a mesh for a FA state variable domain

In this section, we consider building a mesh to cover a domain of FA state variables applied for neutron cross-section calculations. If K is the space dimension of the FA state variables, a domain of FA state variables is usually described by inequalities

$$x_k^{\min} \leqslant x_k \leqslant x_k^{\max}, \quad k = 1, \ldots, K$$

forming a multi-dimensional parallelepiped. Scaling the variables the parallelepiped is transformed into the unit cube. Thus, a problem of mesh generation for the state variable domain is reduced to a problem of constructing a mesh, which covers uniformly the unit multi-dimensional cube.

It is generally believed that the most uniformly distributed mesh for a unit cube is a regular cubic grid, containing N^K points with the coordinates

$$\left\{\frac{i_1 + 1/2}{N}, \frac{i_2 + 1/2}{N}, \ldots, \frac{i_K + 1/2}{N}\right\},$$

where $i_1,\ldots,i_K$ independently take the values $0,1,\ldots,N-1$.

A sample of the cubic grid with 16 mesh points for a two-dimensional cube is shown in Fig. 1(a). However, the cubic grid is optimal only in the one-dimensional case. If the dimension of the cube increases, uniform properties of the cubic grid rapidly decrease. A proof of this statement has been given by Sobol' as far back as 1957 (Sobol', 1957). Let us consider an example taken from Sobol' and Statnikov (1981) to illustrate it. One may compare the cubic grid shown in Fig. 1(a) with the mesh presented in Fig. 1(b). In both cases, each of the 16 cubic cells contains one mesh point, so it seems that the uniformities of the two meshes are approximately equal. Let us consider a problem to approximate a function $f(x_1,x_2)$ by the method of least squares. Then, let us assume that the function does not depend on one variable,

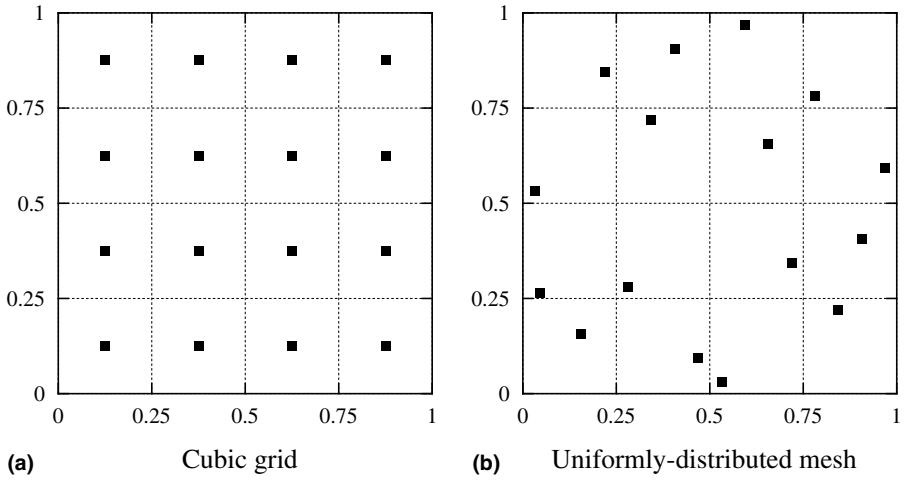


Fig. 1. Examples of the two-dimensional meshes with 16 mesh points: (a) cubic grid, (b) uniformly distributed grid.

i.e. $f(x_1,x_2) \approx f(x_1)$. If a cubic grid is used to compute function values we have only 4 values of the function, which are each repeated 4 times. If the mesh shown in Fig. 1(b) is applied, we have 16 function values, which give a much better function representation and result in a better function approximation.

In the multi-dimensional case, the cubic grid is even worse, because the loss of information is even greater: we compute N^K mesh points and obtain only $N^{1/K}$ different function values. This example of the cubic grid being the worst case is quite realistic, because neutron cross-sections depend strongly on some state variables and weakly on others. Moreover, different cross-sections have different dependencies, so we can not optimize the mesh in consideration of the neutron cross-section dependencies.

The most famous of the uniformly distributed sequences are the quasi-random sequences of Sobol' (1967). A definition and an analysis of these sequences is outside the scope of this paper; an interested reader is referred to the original papers and monographs (Sobol', 1967, 1969; Sobol' and Statnikov, 1981). A short introduction and referencies are given also in Section 7.7 of (Press et al., 1992). We only want to note that the first 2^i points of Sobol's sequences, where i is an arbitrary integer number, have the best uniformity property. Thus, it is recommended that sequences with a number of points equal to 2^i are used. An efficient algorithm to compute Sobol' sequences was developed by Antonov and Saleev (1979), a computer code in FORTRAN implementing this algorithm is presented in Bratley and Fox (1988).

In the case of building a mesh for FA state variables, we have the problem of combining a one-dimensional mesh for burnup, which is defined by a burnup code user or automatically selected by a burnup code, with a multi-dimensional mesh applied in branch calculations. We propose to use a simple combination of the specified one-dimensional burnup mesh with the uniformly distributed mesh generated by a Sobol' sequence. An algorithm for the mesh generation is described as follows:

(1) A number of burnup mesh points N_{burnup} are estimated.
(2) A number of branch calculations at each burnup step J_{dev} are selected. It is recommended, that the total number of the branch calculations $N_{\text{dev}} = J_{\text{dev}} \times N_{\text{burnup}}$ is equal to 2^i, where i is an arbitrary integer number.
(3) A uniformly distributed Sobol' sequence $\{(x_1^n, x_2^n, \ldots, x_{K-1}^n), \quad n = 1, \ldots, N_{\text{dev}}\}$ is computed, where $(K-1)$ is the space dimension of the FA state variables except burnup.
(4) J_{dev} points of the Sobol's sequence are used for branch calculations at each time step of the burnup calculation.

3. Combined interpolation/approximation procedure for neutron cross-sections

In the results of FA calculations, two sets of neutron cross-sections are generated:

- base neutron cross-sections $\Sigma^{\text{base}}(B_n)$, $n = 1,\ldots,N_{\text{burnup}}$, which depend only on burnup;

- branch cross-sections $\Sigma^{\text{dev}}(B_n, x_1^{nj}, x_2^{nj}, \ldots, x_{K-1}^{nj}), \quad n = 1, \ldots, N_{\text{burnup}}; j = 1, \ldots, J_{\text{dev}}$, which depend on the all FA state variables.

The burnup dependence of the base neutron cross-sections is described by a cubic spline. To compute a cubic spline we use the package PCHIP (Fritsch and Carlson, 1980) of the SLATEC library (Buzbee, 1984). The program computes a piecewise cubic Hermite interpolant of the given data. To be used in a neutron cross-section library, the Hermite representation is converted into a piecewise polynomial representation, which is more efficient in this case. A description of the one-dimensional cubic spline interpolation is given in many numerical analysis textbooks, for example in Kahaner et al. (1989) and Press et al. (1992).

The two sets of neutron cross-sections are applied in the multi-dimensional approximation. To decrease their functional dependence on burnup we form a set of deviations of the neutron cross-sections from the base cross-sections as

$$\Delta\Sigma^{\text{dev}} = \begin{cases} \Sigma^{\text{dev}}(B_n, x_1^{nj}, x_2^{nj}, \ldots, x_{K-1}^{nj}) - \Sigma^{\text{base}}(B_n), & n = 1, \ldots, N_{\text{burnup}}; j = 1, \ldots, J_{\text{dev}} \\ 0 = \Sigma^{\text{base}}(B_n) - \Sigma^{\text{base}}(B_n), & n = 1, \ldots, N_{\text{burnup}} \end{cases} \tag{1}$$

The deviations are approximated by multi-dimensional polynomials using the least squares method. Before describing the approximation procedure the basic notation of regression analysis is introduced (Draiper and Smith, 1981).

3.1. Basic notation of regression analysis

Let us consider the problem of building a functional relationship between a dependent variable y, called a *response*, and independent variables $x_1, x_2, \ldots, x_M$, called *regressors*. Linear regression analysis considers only linear models as

$$y = b_0 + b_1 x_1 + \cdots + b_M x_M + error, \tag{2}$$

where b_m is the unknown model coefficients, *error* is the error of the regression model.

A set of N data points is given containing the response and the regressors as

$$x_{n1}, x_{n2}, \ldots, x_{nM}, y_n, \quad n = 1, \ldots, N.$$

The problem of finding coefficients of the linear model (2) is formulated in terms of the *least squares method*: to find a set of coefficients, which minimizes a square norm of the model error vector, i.e. find $b \in \mathbb{R}^{M+1}$, such that $\|Xb - y\|_2^2$ is minimal, where

$$X = \begin{vmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1M} \\ 1 & x_{21} & x_{22} & \cdots & x_{2M} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{N1} & x_{N2} & \cdots & x_{NM} \end{vmatrix} \in \mathbb{R}^{(M+1)\times N},$$

where $y = col\{y_1, y_2, \ldots, y_N\} \in \mathbb{R}^N$ is the response vector, $b = col\{b_0, b_1, b_2, \ldots, b_M\} \in \mathbb{R}^{M+1}$ is the vector of the unknown coefficients.

Several algorithms have been developed to solve the least squares problem (Trefethen and Bau, 1997). We use an algorithm based on *QR*-factorization (Miller, 1992), implemented in FORTRAN 90 module LSQ by Miller (2000).

The resulting vector of the coefficients b minimizes the *sum of square errors*

$$SS_E = \|y - \hat{y}\|_2^2,$$

where $\hat{y} = Xb$ is the predicted response.

The number degrees of freedom associated with the residual error is equal to the number of data points N minus the number of model coefficients including the intercept $M + 1$. The *mean squared error* of the model is defined as the sum of the squared error divided by the error degrees of freedom

$$MS_E = SS_E/(N - M - 1).$$

The mean squared error is equal to the unbiased estimator of the error variance σ^2. The square root of the model-dependent error variance σ is used as an estimator for the model-dependent "standard deviation" and is called the *standard error of the regression model*.

In the same way, the *regression sum of squares*

$$SS_R = \|\hat{y} - \bar{y}\|_2^2,$$

where $\bar{y}$ is the average of all the responses; and the *regression mean square*

$$MS_R = SS_R/(N - 1),$$

where $N - 1$ is the number degrees of freedom of the regression model, are defined.

3.2. Tests of significance of the regression model and the individual coefficients

By applying the least squares technique we can calculate regression coefficients of an arbitrary linear model. However, this does not tell us if the proposed model or computed coefficients actually have statistical significance. In other words, does the model we defined have any meaning comparing with the error in the data? Does a regression coefficient for a given variable have any significance or it can be dropped from the model without any loss of model accuracy? To answer these questions, tests of significance of the regression model and the individual regression coefficients are developed.

To estimate the significance of the regression model statisticians introduce a so-called *null hypothesis*, which can be formulated as "the null hypothesis is true if there is no linear relationship between the response and the regressors". It can be expressed mathematically as

$$H_0 : b_1 = b_2 = \cdots = b_M = 0.$$

The *rejection of the null hypothesis* can be defined as

$$H_1 : b_m \neq 0 \quad \text{for at least one } m.$$

If the null hypothesis is not true, at least one independent variable significantly contributes to the linear model. Thus, we can conclude that a functional relationship exists between the response and at least one of the variables. The test of significance of the regression model is performed as an analysis-of-variance procedure by calculating the ratio of the regression mean square to the mean square error as

$$F = MS_{\mathrm{R}}/MS_{\mathrm{E}}.$$

The null hypothesis is rejected if the computed F-criterion is greater than the corresponding critical value $F_{\mathrm{crit}} = F_{\alpha,M,N-M-1}$ of the F-distribution for a given significance level α with M and $N - M - 1$ degrees of freedom. The significant level α stands for the probability that the null hypothesis is true, i.e. the model is not significant. Usually significance levels of 10%, 5% and 1% are used to determine the critical value F_{crit}, where a decreasing significance level indicates a higher confidence in the model.

In a similar way, the null hypothesis H_{0m} and the rejection of the null hypothesis H_{1m} for the individual regression coefficients are defined:

$$H_{0m} : b_m = 0,$$

$$H_{1m} : b_m \neq 0.$$

If the null hypothesis H_{0m} is rejected, the corresponding coefficient b_m significantly contribute to the model. If H_{0m} can not be rejected, the corresponding variable can be eliminated from the model equation. To assess the significance of an individual coefficient two regression models are considered: the model with coefficients $\{b_0,b_1,\ldots,b_m,\ldots,b_M\}$, which includes the term with the coefficient b_m and the model without this term with the coefficients $\{b_0,b_1,\ldots,b_{m-1},b_{m+1},\ldots,b_M\}$. To test the null hypothesis H_{0m} the individual $F(b_m)$-criterion is computed as

$$F(b_m) = [SS_{\mathrm{R}}(\text{with } b_m) - SS_{\mathrm{R}}(\text{without } b_m)]/MS_{\mathrm{E}}(\text{with } b_m), \tag{3}$$

where SS_{R}(with b_m) is the regression sum of squares of the model with the coefficient b_m, SS_{R}(without b_m) is the regression sum of squares of the model without the coefficient b_m, MS_{E}(with b_m) is the mean squared error of the model with the coefficient b_m.

The computed value $F(b_m)$ is compared with the corresponding critical value F_{crit}. If $F(b_m)$ is larger than F_{crit}, the null hypothesis is rejected and the variable with b_m is left in the model, otherwise the null hypothesis is accepted and the corresponding variable can be eliminated from the model.

3.3. Forming an optimal approximating polynomial

To generate a polynomial model describing neutron cross-section dependencies on FA state variables we need to select the polynomial terms, which make significant contributions. Analysing one-dimensional dependency for each variable we can select an order of polynomial, describing the dependence with acceptable accuracy.

In real-life LWR problems, macro cross-sections depend on at least four FA state variables and the problem of optimal polynomial selection can not be treated by a trial and error approach. For example, for five FA state variables a 4th order polynomial has 126 terms. Different polynomial terms make different contributions to the model, and we would like to select only those terms, which are significant. A method for selecting an optimal subset of the polynomial terms to approximate cross-section dependencies on FA state variables is given in this section.

Considering one-dimensional dependencies of cross-sections on FA state variables we can estimate a maximum order of polynomial for each FA state variable. As a result, a multi-dimensional polynomial can be constructed as a tensor-product of the one-dimensional polynomials. Assuming that cross-sections depend on three variables $\{z_1,z_2,z_3\}$, and the polynomial orders for these variables are {5,2,3}, then the polynomial terms are constructed as

$$x_m(z_1,z_2,z_3) = P_i(z_1) \times P_j(z_2) \times P_k(z_3), \text{ for } 0 \leqslant i \leqslant 5,\ 0 \leqslant j \leqslant 2,\ 0 \leqslant k \leqslant 3;\ i+j+k \leqslant 5,$$

where $P_i(z)$ is the Legendre polynomial of order i.

Application of orthogonal polynomials, such as Legendre polynomials, is recommended, because this decreases the condition number of matrices in the least squares method and make easier the selection of optimal polynomial terms.

The selection of polynomial terms, which optimally describe the cross-section dependencies, is performed using regression analysis tools. First of all, a criterion of optimality is formulated. We would like to describe the cross-section dependencies within a given accuracy. As an accuracy criterion we can use a relative standard error of the regression model defined as

$$\tilde{\sigma}_{\mathrm{E}} = \sqrt{MS_{\mathrm{E}}} \times 100/\bar{y}. \tag{4}$$

The standard error usually decreases if the number of polynomial terms is increased. On the other hand, to minimize the computing time of the model and the number of data points used to compute the model regression coefficients, we would like to minimize the number of polynomial terms in the model. The selection of the optimal polynomial, which, on one hand, provides the model accuracy and, on the other hand, has a minimum number of terms, is our task.

An optimal solution of this problem requires calculation of all possible regression models to find the best. The number of the possible subsets of one or more variables (polynomial terms) out of M is $(2^M - 1)$. Thus, due to a limitation on computing time, exhaustive search algorithms performing the optimal subset selection are recommended for a number of variables, which does not exceed 20 (Miller, 2002). Because in our problems, we have hundreds of polynomial terms, we did not consider these algorithms in this work. Instead, we decided to apply algorithms, which can not guarantee the optimal model, but can provide a model which is close to the optimal. Such algorithms, developed in regression analysis include *forward selection, backward elimination, stepwise regression* and some others, which are not discussed in this paper. Detailed descriptions of these algorithms can be found in Draiper and Smith (1981) and Miller (2002); below we describe only the basic ideas underlying them.

In the *forward selection* algorithm, we start with a model containing no regressors apart from the intercept. New regressors are added to the model one at a time and the individual $F(b_m)$ criterion is used to decide if the additional regressor actually improves the model. The first regressor variable we select is the one leading to the highest $F(b_m)$ value for the models with one regressor and the intercept. The forward regression uses a threshold value for the lowest possible $F(b_m)$, usually called F_{in}, which determines that the regressor is significant enough to be included into the model. At the following step we select a new regressor with the highest $F(b_m)$ value for the model with two variables. The procedure is continued until the model satisfies the user given criteria of accuracy or there are no variables having $F(b_m)$ values higher than the critical value F_{in}.

The *backward elimination* method works in the exactly opposite direction to forward selection. The model is started with the equation, which includes all possible regressors. Variables are eliminated from the model using the given elimination criterion F_{out}. If the computed value of $F(b_m)$ is less than F_{out}, the variable is dropped from the model.

The *stepwise regression* method is a combination of these two approaches. As in the forward selection method, a model is started with the equation, which contains only the intercept, and one variable is added. Then, a second variable with the maximum value of $F(b_m)$ is added into the model. For the model with two variables the individual criteria $F(b_m)$ for both variables are computed. The values $F(b_m)$ are compared with the elimination criterion F_{out}. The variables are left in the model or eliminated on the results of these tests. A test of the "least valuable" regressor is performed at each step of the procedure. If a variable is eliminated, the regression equation is updated considering all the variables, which are left. Variables, which are not included in the model, are tested using the inclusion criterion F_{in}. If a variable is added, we return to the elimination test. The procedure is terminated if the given model accuracy is reached or if there are no variables left, which pass the inclusion test F_{in}.

The described subset selection algorithms are implemented in many statistical analysis tools, such as SPSS, Statistica and statistical toolbox of the Matlab. We are using the SUBSET module, written by Miller (2001) in FORTRAN-90.

4. Approximation of two-group neutron cross-sections of a VVER fuel pin cell

The described interpolation/approximation procedure is demonstrated on the two-group neutron cross-sections of a VVER fuel pin cell. The three zones of fuel, cladding and coolant have the radii 0.386, 0.4582, 0.6694 cm. Nuclear concentrations of the cell materials are given in Table 1. The fuel contains equilibrium concentrations of xenon and iodine. The power density of the cell is 108 W/cm^3. The collision probability code UNK (Tsybulsky and Davidenko, 2002) is used to compute the two-group neutron cross-sections. The cross-sections depend on the following parameters:

- b – burnup [0, 60] MWt × day/kgU;
- ρ – coolant density [0.25, 1] g/cm^3;

Table 1
Initial material composition of the VVER fuel pin cell under the nominal conditions ($b = 0$ MWt × day/kgU, $\rho = 0.72$ g/cm^3, $T_c = 575$ K, $T_f = 950$ K, $c_B = 500$ ppm)

Material	Isotope	Concentration, (atom/barn-cm)
Uranium oxide fuel	U-235	8.73700E-04
	U-238	1.87440E-02
	O-16	3.92350E-02
	Xe-135	9.74049E-09
	I-135	2.07109E-08
Cladding	Zr-nat	4.23E-03
Coolant	H-1	4.81354E-02
	O-16	2.40677E-02
	B-10	3.96154E-06
	B-11	1.61071E-05

- T_c – coolant temperature [293, 603] K;
- T_f – fuel temperature [293, 1793] K;
- c_B – boron concentration [0, 1500] ppm.

In the approximation procedure, scaled variables defined as

$$\xi = (2x - x_{\max} - x_{\min})/(x_{\max} - x_{\min})$$

are used. The list of cross-sections includes the macro cross-sections

$$\left\{\Sigma_{tr1}, \Sigma_{tr2}, \Sigma_{a1}, \Sigma_{a2}, \nu\Sigma_{f1}, \nu\Sigma_{f2}, \Sigma_{f1}, \Sigma_{f2}, \Sigma_s^{1->2}\right\},$$

the cell multiplication factor $k_{\inf}$ and the thermal group absorption cross-sections of xenon σ_{a2}^{Xe-135} and samarium σ_{a2}^{Sm-149}. The burnup step size of the calculation is equal to 0.5 MWt × day/kgU. The burnup calculation is performed under the following nominal conditions of the cell: $\rho = 0.72$ kg/cm^3, $T_c = 575$ K, $T_f = 950$ K, $c_B = 500$ ppm. Four branch calculations are performed at each burnup step. A Sobol' uniformly distributed sequence is used as a mesh for the branch calculations. Two two-dimensional projections of this mesh are shown in Fig. 2.

The dependence of the base cross-sections on burnup is interpolated by a cubic spline. The burnup dependence of the base absorption cross-sections of the fast and thermal groups are shown in Fig. 3. To compute the spline interpolant 64 burnup points are used; the remaining burnup points form a control data set, which is applied to test the accuracy of the cubic spline interpolation. Mean squared and maximum errors computed on the control data set are given in Table 2. The results show that for most applications the accuracy of the spline interpolation is more than enough.

Optimal multi-dimensional polynomials to approximate the dependencies of the deviations (1) on the cell state variables are generated by the stepwise regression algorithm. The accuracy criterion (4) is equal to 0.05%. A tensor-product polynomial basis is constructed using Legendre polynomials of orders {6,6,5,4,4} for the cell state variables $\{b,\rho,T_c,T_f,c_B\}$. The orders of the one-dimensional polynomials are estimated from the results of one-dimensional approximations. The number of terms

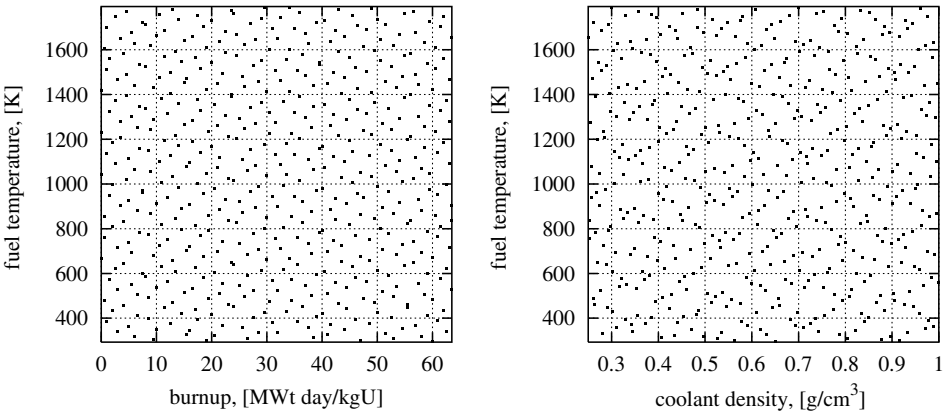


Fig. 2. Two-dimensional projections of the mesh used in the calculations.

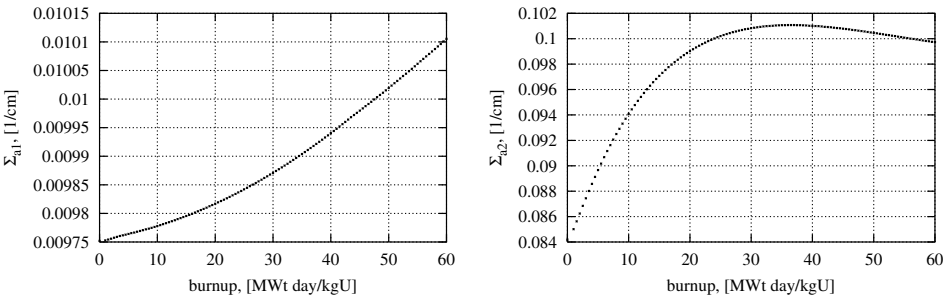


Fig. 3. Examples of the dependencies on burnup of the base macro cross-sections.

Table 2
Mean squared Δ^{sqrt} and maximum Δ^{max} errors of the cubic spline interpolation of the dependency of the base cross-sections on burnup

Error (%)	Σ_{tr1}	Σ_{tr2}	Σ_{a1}	Σ_{a2}	$\nu\Sigma_{f1}$	$\nu\Sigma_{f2}$	Σ_{f1}	Σ_{f2}	$\Sigma_s^{1->2}$	k_{inf}	σ_{a2}^{Xe}	σ_{a2}^{Sm}
Δ^{sqrt}	0.000	0.000	0.001	0.010	0.006	0.018	0.006	0.016	0.000	0.006	0.003	0.003
Δ^{max}	0.001	0.001	0.002	0.093	0.039	0.133	0.034	0.109	0.002	0.038	0.025	0.021

Table 3
Powers of the terms of the five-dimensional approximating polynomial for the deviation of the fast group absorption cross-section $\Delta\Sigma_{a1}$

Power of the polynomial terms																	
b	0	0	1	0	0	1	0	0	1	1	0	0	0	0	0	0	0
ρ	0	1	0	0	2	2	4	1	0	1	0	0	1	3	2	0	1
T_c	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
T_f	0	2	1	3	1	0	0	0	0	0	2	0	1	0	0	1	0
c_B	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0

Table 4
Powers of the terms of the five-dimensional approximating polynomial for the deviation of the thermal group absorption cross-section $\Delta\Sigma_{a2}$

Power of the polynomial terms																									
b	0	3	4	0	1	2	4	1	0	0	4	0	0	2	2	1	0	0	0	2	3	2	0	0	0
ρ	0	1	1	1	0	1	0	1	1	0	0	5	0	0	0	0	0	1	0	2	0	1	0	2	1
T_c	0	1	0	3	3	0	1	2	0	3	0	0	0	2	0	1	1	1	0	0	1	1	1	0	0
T_f	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	2	0	0	0	0	0	1
c_B	0	0	0	0	0	1	0	0	2	0	0	0	2	0	1	1	0	1	0	0	0	0	1	1	0
b	3	1	2	1	0	2	1	1	0	2	1	2	1	1	0	0	0	1	0	0	1	0	0	0	0
ρ	0	0	0	1	4	1	2	0	1	0	1	0	0	0	0	3	0	0	1	1	1	2	0	0	1
T_c	0	2	0	0	0	0	0	0	2	1	1	0	0	0	2	0	0	1	1	0	0	0	1	0	0
T_f	0	0	1	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0
c_B	0	0	0	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1	0	0	0	1	0

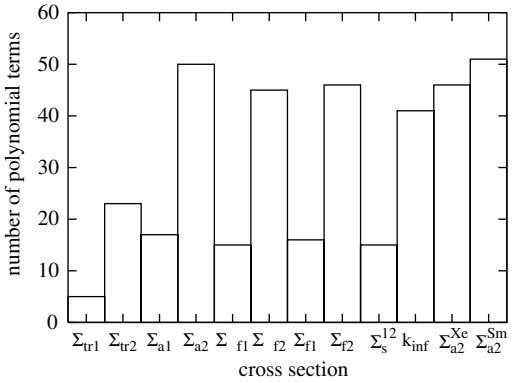


Fig. 4. The number of terms of the approximating polynomials for the given cross-section set.

in the polynomial basis is equal to 448. The number of points in the cross-section deviation set (1) is equal to 640: 128 points are the results of the base burnup calculation and 512 points are computed in the branch calculations. In Tables 3 and 4 the powers of the one-dimensional polynomials forming the approximating polynomials for the fast and thermal absorption cross-sections are shown. The polynomial for the absorption cross-section contains 17 terms for the fast group and 51 terms for the thermal group. The numbers of the polynomial terms for all the cross-sections are shown in Fig. 4. On average less than 20 terms are used in the approximation of the fast group cross-sections and about 50 terms are needed for thermal group cross-sections.

To decrease the computing time of the cross-section evaluation all the polynomial terms used in the approximation of the different cross-sections are grouped into a global approximating polynomial. In the cross-section evaluation, the terms of the global polynomial are computed only once for each point of the cell state variables.

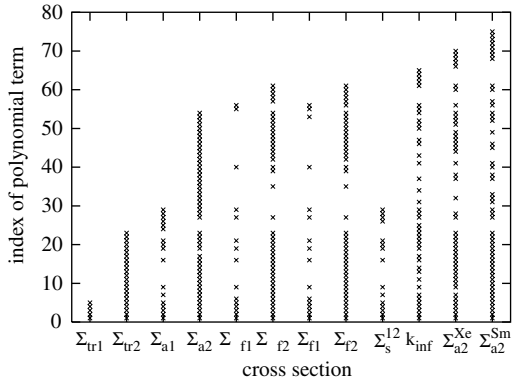


Fig. 5. Indices of the polynomial terms of each cross-section in the global approximating polynomial.

Table 5
Mean squared Δ^{sqrt} and maximum Δ^{max} errors of the polynomial approximation computed on the initial data set

Error (%)	Σ_{tr1}	Σ_{tr2}	Σ_{a1}	Σ_{a2}	$\nu\Sigma_{f1}$	$\nu\Sigma_{f2}$	Σ_{f1}	Σ_{f2}	$\Sigma_s^{1->2}$	k_{inf}	σ_{a2}^{Xe}	σ_{a2}^{Sm}	k_{inf}^{Σ}
Δ^{sqrt}	0.05	0.05	0.04	0.05	0.05	0.05	0.05	0.05	0.04	0.05	0.05	0.05	0.05
Δ^{max}	0.19	0.84	0.21	0.28	0.25	0.24	0.20	0.25	0.51	0.26	0.25	0.20	0.23

Table 6
Mean squared Δ^{sqrt} and maximum Δ^{max} errors of the polynomial approximation computed on the control randomly generated data set

Error (%)	Σ_{tr1}	Σ_{tr2}	Σ_{a1}	Σ_{a2}	$\nu\Sigma_{f1}$	$\nu\Sigma_{f2}$	Σ_{f1}	Σ_{f2}	$\Sigma_s^{1->2}$	k_{inf}	σ_{a2}^{Xe}	σ_{a2}^{Sm}	k_{inf}^{Σ}
Δ^{sqrt}	0.05	0.05	0.04	0.06	0.05	0.05	0.05	0.05	0.04	0.05	0.05	0.06	0.06
Δ^{max}	0.25	0.78	0.24	0.61	0.30	0.28	0.32	0.25	0.57	0.23	0.27	0.31	0.56

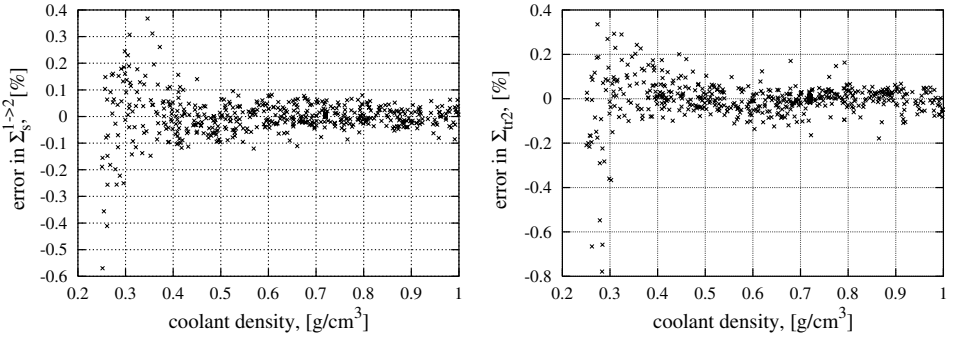
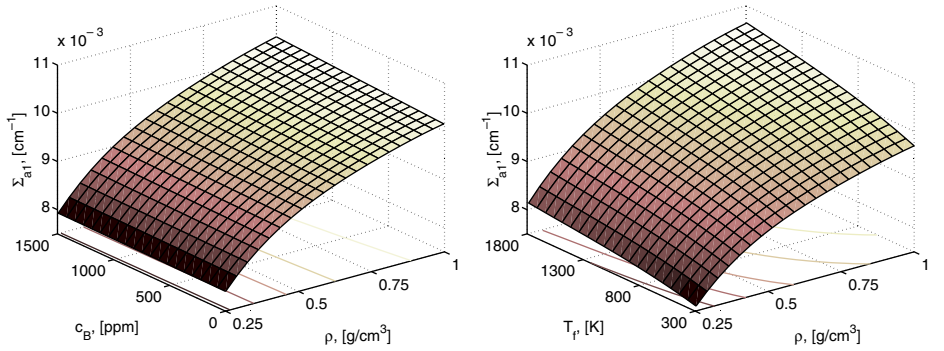
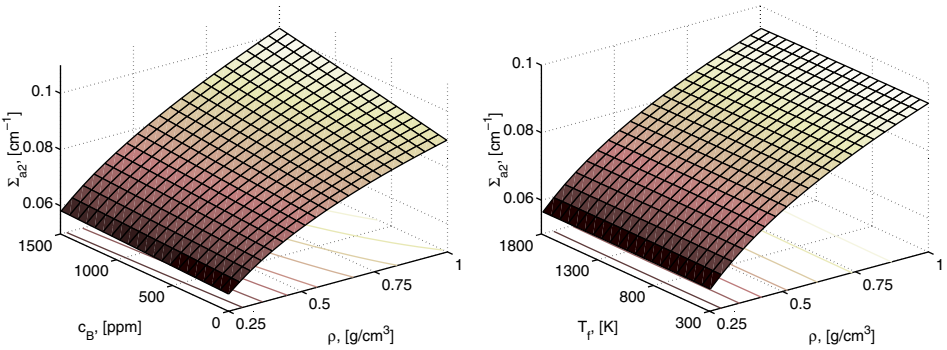


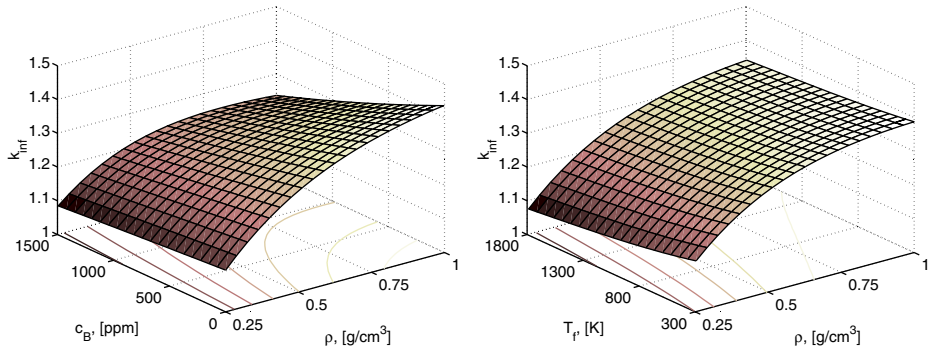
Fig. 6. Errors of the cross-section approximation as a function of coolant density: (a) scattering cross-section $\Sigma_s^{1->2}$, (b) thermal transport cross-section Σ_{tr2}.



(a) fast group absorption cross section Σ_{a1}



(b) thermal group absorption cross section Σ_{a2}



(c) multiplication factor k_{inf}

Fig. 7. Two-dimensional projections of the dependencies of the neutron cross-sections: (a) fast group absorption cross-section Σ_{a1}, (b) thermal group absorption cross-section Σ_{a2}, (c) multiplication factor k_{inf}. Figures on the left – the dependencies on the coolant density and boron concentration; figures on the right – the dependencies on the coolant density and fuel temperature.

Then, the individual cross-section is computed as a scalar product of the global approximating polynomial terms on a vector of the polynomial coefficients. In Fig. 5, a cross marks terms of the global polynomial, which is used in the approximation of each cross-section. The number of terms of the global polynomial is less than 80 for the given cross-section set.

The accuracy of the approximation procedure is tested on two data sets: on the initial set, which is used in the approximation procedure and on a control data set being computed in the branch calculations on randomly generated mesh points. The burnup meshes and respectively the base cross-sections are the same in both data sets. In Tables 5 and 6 errors of the approximation on both sets are given. Besides the cross-sections, the last column k_{inf}^{Σ} contains an error in the cell multiplication factor computed using the approximated cross-sections. For all the cross-sections mean squared errors do not exceed 0.065%.

A comparison of the results given in Tables 5 and 6 shows, that the approximation errors computed on the initial data set are representative and can be used as a measure of approximation accuracy. The dependencies of the approximation errors for the scattering cross-section $\Sigma_s^{1\to 2}$ and the thermal transport cross-section Σ_{tr2} as functions of coolant density are shown in Fig. 6. The maximum errors of the approximation correspond to low values of the coolant density, which can only occur under severe accident reactor conditions. For the simulation of severe reactor accidents, the obtained accuracy of the approximation is considered as acceptable.

Computing time of the approximation procedure for the considered data set is less than one minute on PC with processor AMD 1900+.

Concluding this section, Fig. 7 demonstrates the complexity of the computed approximation function showing two-dimensional projections of the dependencies of the absorption macro cross-sections Σ_{a1} and Σ_{a2}, and the cell multiplication factor k_{inf}. The two-dimensional dependencies are computed at zero burnup for nominal values of the other FA state variables. These figures show that the approximated dependencies are complicated functions of the state variables and the dependencies are different for different cross-sections. Thus, the selection of the form of the approximating polynomial considered in this paper is actually not a trivial task.

5. Conclusions

A combined interpolation/approximation procedure to describe the dependencies of few-group neutron cross-sections on burnup and thermal-hydraulics parameters of a cell is proposed in this paper. The neutron cross-section is presented as a sum of two terms: the base cross-section, which depends only on burnup and is computed under the nominal cell conditions, and the deviation, which depends on all the cell parameters. The dependence of the base cross-sections on burnup is interpolated by a cubic spline. The deviation dependencies are approximated by a multi-dimensional polynomial. The main feature of the proposed procedure is the generation of an optimal approximating polynomial, which describes the deviation dependencies within a user given tolerance. Optimality means that the number of

terms forming the approximating polynomial is minimal for the given accuracy of approximation. This problem is solved by regression analysis techniques: terms of the approximating polynomial are selected from an initial polynomial basis using the stepwise regression algorithm.

The proposed procedure is demonstrated by building the dependencies of the two-group neutron cross-sections of a VVER fuel cell as functions of burnup, coolant density, fuel and coolant temperatures and boron concentration. The cross-sections are computed by the collision probability code UNK. The mean squared error of the cubic spline interpolation of the base cross-sections does not exceed 0.02%. Polynomials describing the dependencies of the deviations are constructed using the stepwise regression algorithm. The relative mean squared error of the approximation is specified as 0.05%. This accuracy is provided by five-dimensional polynomials containing less than 20 terms for fast group cross-sections and about 50 terms for thermal group cross-sections. The constructed polynomials are tested on the two data sets: the initial data set and on the control data set, computed in the branch calculations on randomly generated mesh points. The mean squared errors of the polynomial approximation are approximately equal for both data sets. Thus, the initial data set used in the polynomial construction can be also applied in the control of approximation accuracy.

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