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PWR few-group constants parameterization analysis

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ABSTRACT

To provide few-group constants for the assembly-homogenized PWR core neutronics simulation based on the two-step approach, few-group constants parameterization is required by using the discrete relationship between those few-group constants and the assembly state parameters. As numerical methods for both lattice and core calculations have been more and more advanced, few-group parameterization tends to be the main error source for reactor physics calculations. In addition, there are also other effects such as history effect expected to be treated during parameterization process. Currently there are several parameterization methods but there is no clear conclusions drawn on how to select when dealing with new problems or developing new codes. Thus, this study characterized the entire few-group constants parameterization into three main aspects, namely the combination of state parameters, functionalization and attached effects, and developed a common link code named NECP-Lilac to answer those questions. Firstly, by optimizing state parameter combination, error of few-group constants is reduced by half. Secondly, the two most widely employed functionalization methods including linear interpolation and least-square fitting are compared based on typical PWR problems. Linear interpolation is recommended for new reactors since it needs almost no experience on discrete point generation process as long as there are sufficient numbers of them. Least-square fitting is suggested for routine calculations considering the fact that it needs only half discrete points for each state parameter to provide the same precision with linear interpolation. Thirdly to treat the history effect, two methods including macro-correction and micro-depletion are implemented and compared. It has been found that the micro-depletion method can always reduce the corresponding error while the performance of the macro-correction method appears case dependent.

1. Introduction

Traditionally, during design and operation simulation processes, Pressurized Water Reactor (PWR) core is calculated by using the so-called two-step approach (Hébert, 2009; Smith, 1986). Firstly, it is the lattice calculation which provides a neutronic few-group constants library usually on assembly geometry for specific discrete states. These neutronic few-group constants include few-group (usually two-group) macro- and microscopic cross sections, pin-power form factors, discontinuity factors and so on, while these states are represented by state parameters or state variables such as fuel burnup, boron concentration, fuel and moderator temperatures and et al. Secondly, coupled neutron diffusion and thermal-hydraulics are usually carried out for a single- or quarter-assembly homogenized whole core configuration, which may need spatially homogenized and energy group condensed neutronic few-group constants at any possible discrete state. Considering the fact that the discrete state required by the reactor core calculation may be different from the ones provided by the lattice calculation, a process is required to provide a function between those neutronic few-group constants and state parameters based on the discrete points provided by lattice calculations. It is usually named as few-group constant parameterization, or the link process, or cross section model.

Form the implementation point of view, few-group constants parameterization can be separated into three steps. Firstly, a set of parameters that strongly affect the few-group constants should be selected as state parameters to represent the state of the assembly. Traditionally, those selected state parameters consist of fuel burnup (*Bu*), boron concentration (*CB*), relative power density (*Pr*), fuel

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0149-1970/

temperature (*Tf*), moderator temperature (*Tm*), moderator density (ρ), void fraction x_v, neutron spectrum index (*SI*), control rod position (*CR*) and so on. Secondly, instead of directly obtaining a multi-dimensional function between each few-group constant and those state parameters, each of the constants is separated into several components according to their physical affecting mechanism. For example, *Bu* and *CB* are usually combined together to make a joint contribution component, while Tm and Bu are combined together to make another. In this way, both computing effort and storage requirements can be decreased by the avoiding of the dimension curse (Bokov et al., 2012). However, if state parameters cannot be decoupled properly to take into account the coupling of the close related ones, extra error may be introduced. Thirdly, for each component, a functionalization is required by using the discrete points provided by lattice calculation. Traditionally, least-square fitting (Zhang et al., 2005; Mayhu et al., 2006; Boyd et al., 2009) and linear interpolation (Shen, 2004; Huang et al., 2008) are the two widely employed functionalization algorithms, noticing that other algorithms are also investigated (Bokov et al., 2012).

Traditionally, neither lattice nor reactor core calculation techniques are developing research areas. But the errors caused by those two are reduced during the past decades, leaving the few-group constants parameterization as almost an engineering topic, strongly experience dependent and becoming the main error source. In addition, some special effects such as history effect can also be considered in few-group constants parameterization process. The term history effect (Fujita et al., 2014) refers to the difference of neutronic few-group constants between two assembly states which share exactly the same state parameters but experienced different depletion processes starting from exactly the same beginning. It happens mainly due to the dependence of the nuclide density evaluation to the depletion history.

To provide an insight of the link process, and also to provide a tool to evaluate the currently available approaches for specific applications, Nuclear Engineering Computational Physics (NECP) laboratory of Xi'an Jiaotong University has developed a general code named NECP-Lilac (Gao, 2015) (LInk of LAttice code and Core simulator) in an modularized object-oriented manner. The term "general" here refers to that the code leaves a number of options to its users other than fixing them in the source code. In this code, there is no limitation on the type or the number of few-group constants, the type or the number of state parameters, the combination of those state parameters et al. Thus, by using this code, we evaluated different parameterization models. The evaluation results and the conclusions based on typical Pressurized Water Reactor (PWR) are summarized in this paper, mainly in three aspects. First, it is the optimization of the combination of state parameters including *Bu*, *CB* and *Tf*. Second, two functionalization methods, namely the least-square fitting and the multi-dimensional linear interpolation, are developed, compared and analyzed. Third, two history effect treatments namely the macro-correction and micro-depletion methods are implemented, evaluated and compared.

This paper is organized as following. Section 2 introduces the theory of the three evaluations, while Section 3 lists the numerical results based on typical PWR problems. Finally, Section 4 summaries the conclusions.

2. Theoretical model

In this section, after introducing the original and improved combinations of state parameters, the two functionalization methods and the two history effect treatments are described in detail.

2.1. The combination of the state parameters

To avoid direct multi-dimensional functionalization with the curse of dimension, all of the state parameters are usually combined together to provide several terms to be summed and/or multiplied together to obtain the active few-group constants. Considering that *Bu* provides accumulated effect on few-group constants while the others has only instantaneous effects, the most obvious way is to combine *Bu* with each of the others, such as:

$$\Sigma(Bu, CB, Tf, Tm) = f_{\mathrm{Base}}(Bu, CB) + f_{\mathrm{Fuel}}(Bu, Tf) + f_{\mathrm{Moderator}}(Bu, Tm) \quad (1)$$

It is currently widely adopted by many codes such as CASMO/SIMULATE (Studsvik, 2009, 1995), GLORY (Huang et al., 2008), SIMME (Cao, 2013) et al. BTW, it is optional in SIMULATE to combine any three of them together.

The combination of those state parameters can save a lot of computing time and memory. For example, there are 30 burnup steps, 7 boron concentrations, 4 fuel temperatures and 3 moderator temperatures for a very conservative prediction for PWR assemblies. The complete combination of all four demands $30 \times 7 \times 4 \times 3 = 2520$ states to be evaluated by the lattice calculation. As required by Eq. (1), only $30 \times (7 + 4 + 3) = 420$ states would be required.

Actually, the combination and separation depend on whether the coupling between different state parameters is strong or weak. The combination in Eq. (1) neglects the coupling between *CB*, *Tf* and *Tm*. Considering the fact that both *CB* and *Tm* exist in the moderator, the separation of them would introduce extra error. Thus, an alternative one is suggested

$$\Sigma(Bu, CB, Tf, Tm) = f_{\mathrm{Base}}(Bu, CB, Tm) + f_{\mathrm{Fuel}}(Bu, Tf) \quad (2)$$

In contrast to Eq. (1), the combination in Eq. (2) requires $30 \times (7 \times 3 + 4) = 750$ states for the above example to be evaluated by the lattice calculation.

2.2. Functionalization methods

After the determination of combination form and the evaluation of lattice calculation, the discrete relationship between state parameters and component contribution for each term can be obtained as following:

$$\boldsymbol{x}_i \rightarrow f(\boldsymbol{x}_i) \quad (3)$$

where vector $\boldsymbol{x}_i$ refers to the state parameter vector for discrete state $i = 1 \sim n$ and $f(\boldsymbol{x}_i)$ is the corresponding component.

The term functionalization here means to obtain a contentious relationship between vector $\boldsymbol{x}$ and the function $f(\boldsymbol{x})$ by using the n discrete states in Eq. (1). Currently, the most widely used numerical functionalization methods in few-group constants parameterization are the least-square fitting and the multi-dimensional linear interpolation. Here we only describe how to implement them into the code of NECP-Lilac.

2.2.1. Least-square fitting

It is supposed that the function $f(\boldsymbol{x})$ can be approximated by a sum of finite number (L) of polynomials

$$f(\boldsymbol{x}) \approx \sum_{l=0}^{L} c_l \cdot P_l(\boldsymbol{x}) \quad (4)$$

where $P_l(\boldsymbol{x})$ stands for a polynomial of order l, the corresponding

coefficients c_l can be obtained by minimizing the L_2 norm of the following residual in terms of the vector $\boldsymbol{c}$ constructed by c_l:

$$R(\boldsymbol{c}) = \sum_{i=1}^{n} \left[f(\boldsymbol{x}_i) - \sum_{l=0}^{L} c_l \cdot P_l(\boldsymbol{x}_i) \right]^2 \tag{5}$$

Requiring:

$$\frac{\partial R}{\partial \boldsymbol{c}} = 0 \tag{6}$$

yields a linear algebraic equation:

$$\boldsymbol{A}\boldsymbol{c} = \boldsymbol{b} \tag{7}$$

where the entries of coefficient matrix $\boldsymbol{A}$ and the right hand side vector $\boldsymbol{b}$ are respectively

$$a_{jl} = \sum_{i=1}^{n} P_j(\boldsymbol{x}_i) P_l(\boldsymbol{x}_i) \tag{8}$$

$$b_j = \sum_{i=1}^{n} P_j(\boldsymbol{x}_i) f(\boldsymbol{x}_i) \tag{9}$$

Considering the fact that the entry values of the vector $\boldsymbol{x}$ may be very large such as fuel burnup Bu or very small such as void fraction x_v, the value of their polynomials may turn out to be very large or small by magnitudes, which may cause the Eq. (7) ill-conditioned. To overcome this problem, the entries x are normalized before the actual fitting process:

$$\widetilde{x} = \frac{x - x_{av}}{x_{std}} \tag{10}$$

where x_{av} is the average value of x_i:

$$x_{av} = \frac{1}{n} \sum_{i=1}^{n} x_i \tag{11}$$

x_{std} is its standard deviation:

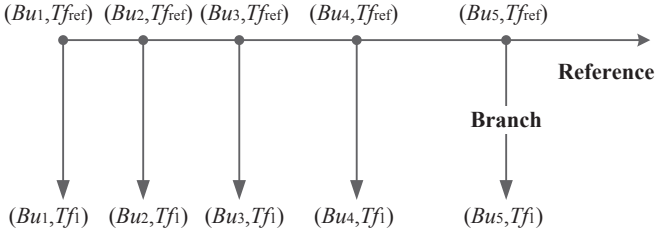


Fig. 1. Branch calculation scheme.

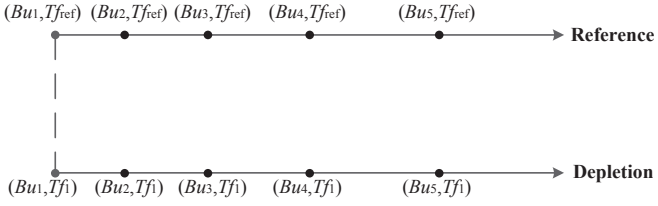


Fig. 2. Depletion calculation scheme.

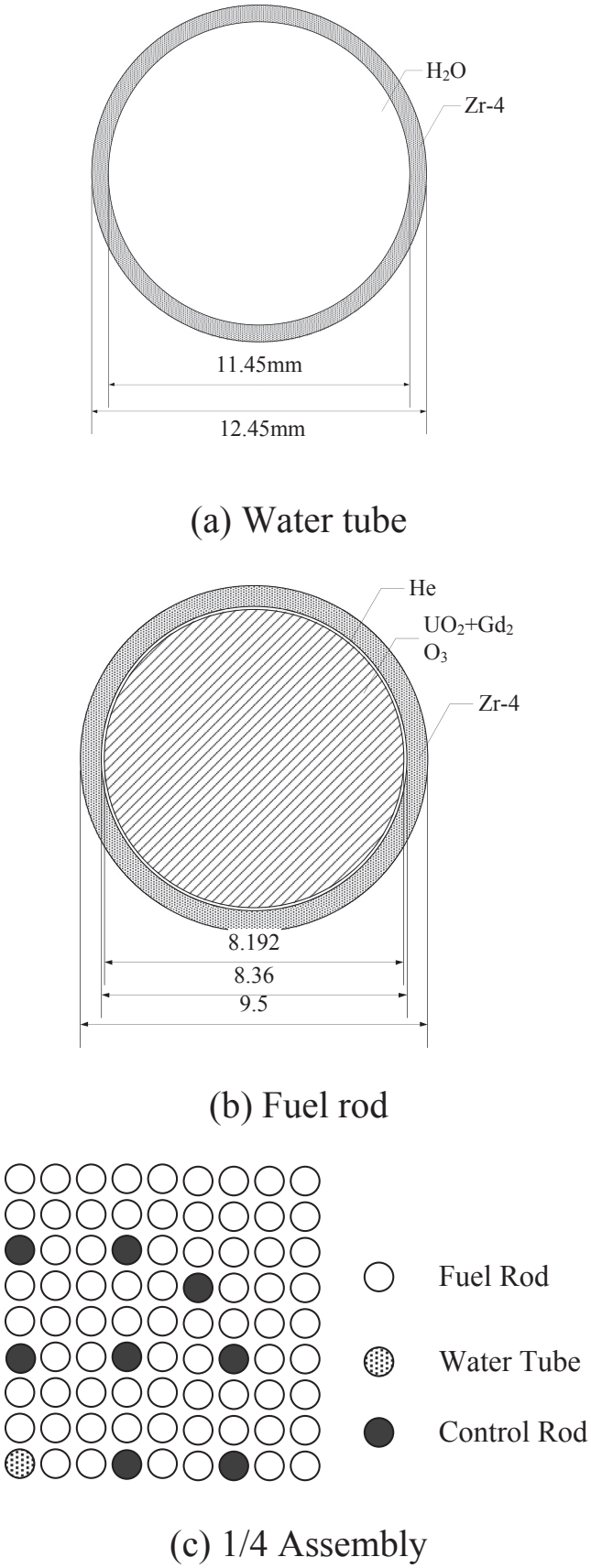


Fig. 3. The typical PWR assembly configuration.

Table 1
Lattice calculation state points.

State Parameter	No. state points	Values
Tf (K)	4	564.12, 723.12, 923.12, 1015.12
Tm (K)	3	566.15, 583.85, 601.55
CB (ppm)	7	0, 200, 500, 1000, 1400, 1700, 2000
Bu (MWd/tU)	52	0, 24, 48, …, 120, 240, 360…, 2520, 3120, 3720…, 14,520, 16,320, 18,120,…, 25,400

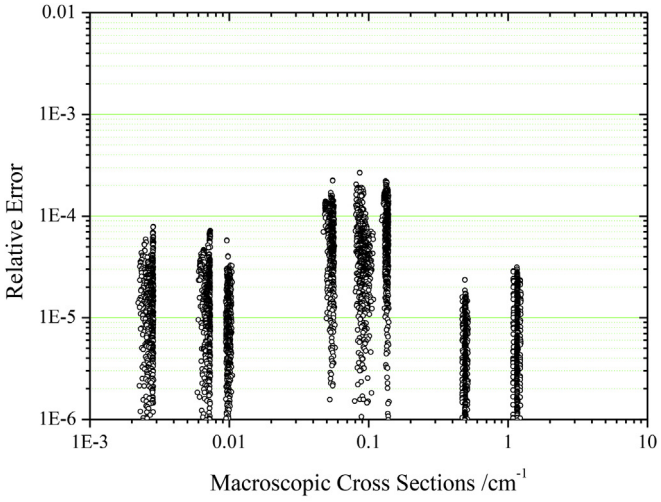
$$x_{std} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_i - x_{av})^2} \tag{12}$$

Once the fitting process is done without the bothering of ill-conditioned equation, the coefficients c_l can be transformed back to the original state parameters. In this way, the precision of the least-square fitting can be guaranteed free from the magnitude of the state parameters.

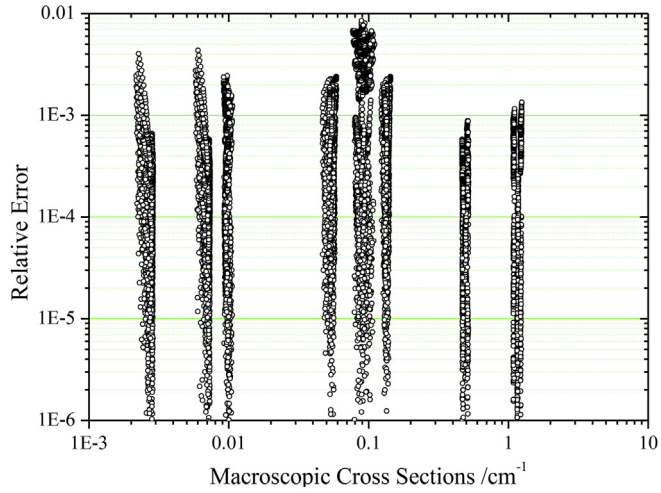
It can be found that *Bu* is a very special parameter compared with the others. It covers a very large domain, usually from 0 to 45,000 MWd/tU or even more. In addition, it affects the few-group constants severely since it indicates the consumption of fissile nuclides and the accumulation of fission products. Consequently, it is very hard to obtain a high precision single polynomial for the entire domain of *Bu*. Low order polynomials cannot describe the shape of the curve, while high order polynomials would cause the Runge's phenomenon (Gautschi, 2012). Thus, the *Bu* domain is usually divided into several segments, and then the least-square fitting is carried out separately one segment after another. It is important to notice that the connection between two adjacent segments has to be guaranteed to avoid non-physical divergences in neutronics and thermal-hydraulics coupling iteration and in critical searching iteration.

2.2.2. Multi-dimensional linear interpolation

Instead of minimizing the L_2 norm of the residual between the polynomial approximation and the active function on the discrete state points, the multi-dimensional linear interpolation method tries to directly connect the state points to make a piece wise linear

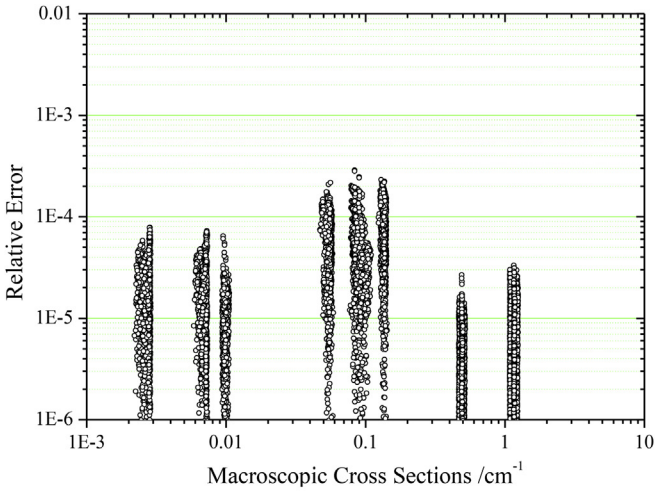


(a) Parameterization error on used points

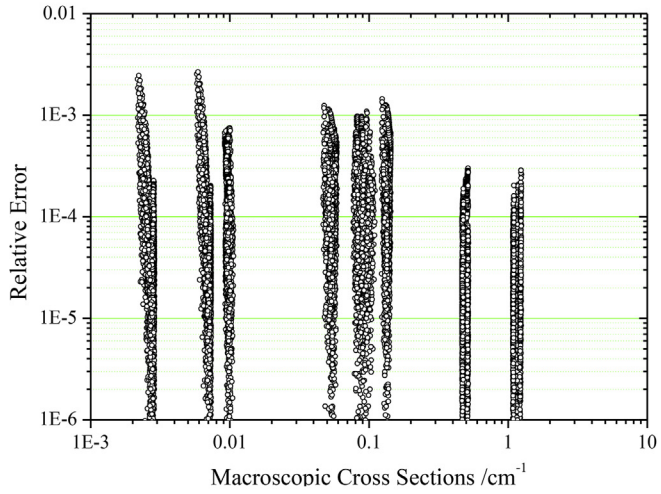


(b) Parameterization error on raw points

Fig. 4. Parameterization errors when *CB* and *Tm* are separated.



(a) Parameterization error on used points



(b) Parameterization error on raw points

Fig. 5. Parameterization errors when *CB* and *Tm* are combined.

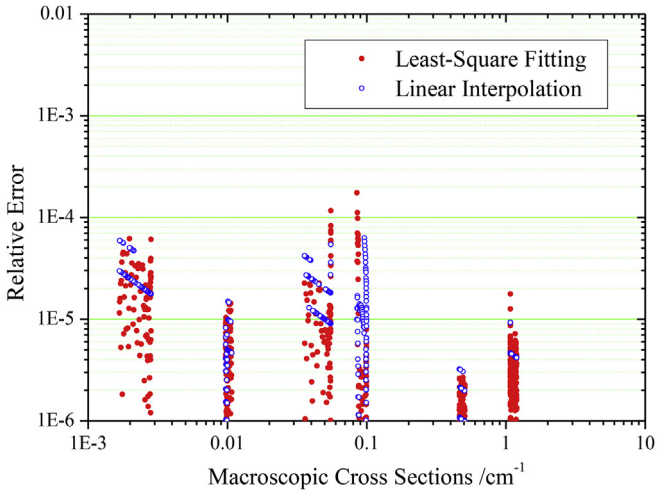
Table 2
Burnup steps.

Segment	Start/GWd tU^{-1}	End/GWd tU^{-1}	Step/GWd tU^{-1}	No. state points
1	0.0000	0.1203	0.02406	5
2	0.1203	2.5263	0.06015	40
3	2.5263	14.5563	0.20050	60
4	14.5563	68.6913	0.60150	91

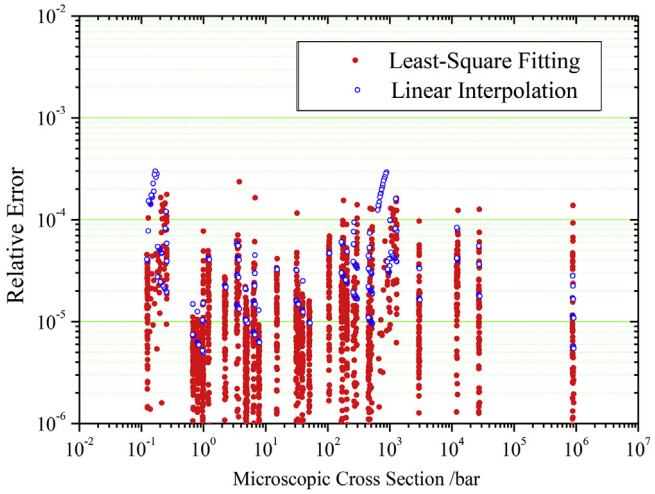
surface to approximate the active function. To obtain the few-group constants for state $\boldsymbol{x}$ with dimension of M, 2^M known state points are required to provide two boundary points in each dimension as $x^m{}_1 \le x^m \le x^m{}_2$ to construct a box or super box that contains the targeted state inside or on the surfaces. Define ${}^m\boldsymbol{x}_1$ and ${}^m\boldsymbol{x}_2$ as the state points with their first m dimensions take the values of $x^1 \sim x^m$ respectively while the $m+1$ dimension are respectively specified as $x^{m+1}{}_1$ and $x^{m+1}{}_2$, and the rest of the dimensions are either $x^{m+2}{}_1 \sim x^M{}_1$ or $x^{m+2}{}_2 \sim x^M{}_2$. The corresponding collections are respectively $\{{}^m\boldsymbol{x}_1\}$ and $\{{}^m\boldsymbol{x}_2\}$, in each of which there are 2^{M-m-1} entries. Also define the sum collection $\{{}^m\boldsymbol{x}\} = \{{}^m\boldsymbol{x}_1\} \cup \{{}^m\boldsymbol{x}_2\}$, which contains 2^{M-m} entries. Consequently, the known 2^M state points belongs to the collection $\{{}^0\boldsymbol{x}\} = \{{}^0\boldsymbol{x}_1\} \cup \{{}^0\boldsymbol{x}_2\}$, and the targeted state point belongs to a single entry collection $\{{}^M\boldsymbol{x}\}$. Based on these definitions, the multi-dimensional linear interpolation becomes how to obtain the few-group constants contributions sequentially for state collections $\{{}^0\boldsymbol{x}\}, \{{}^1\boldsymbol{x}\}, \ldots, \{{}^m\boldsymbol{x}\}, \ldots, \{{}^M\boldsymbol{x}\}$. For each level m, the known collection $\{{}^{m-1}\boldsymbol{x}\}$ is firstly divided into $\{{}^{m-1}\boldsymbol{x}_1\}$ and $\{{}^{m-1}\boldsymbol{x}_2\}$. Then $f({}^m\boldsymbol{x})$ can be obtained:

$$f({}^m\boldsymbol{x}) = f({}^{m-1}\boldsymbol{x}_1) + [f({}^{m-1}\boldsymbol{x}_2) - f({}^{m-1}\boldsymbol{x}_1)]\frac{x^m - x^m_1}{x^m_2 - x^m_1} \tag{13}$$

It can be found that the above process can adapt to problem with any number of dimensions. And also it can be proved that the sequence of the state parameters within the vector $\boldsymbol{x}$ does not affect the final result of $f(\boldsymbol{x})$. In addition, it is worth to notice that the combined linear pieces are not smooth at the known state points which may be required during transient simulations (Liao, 2002).

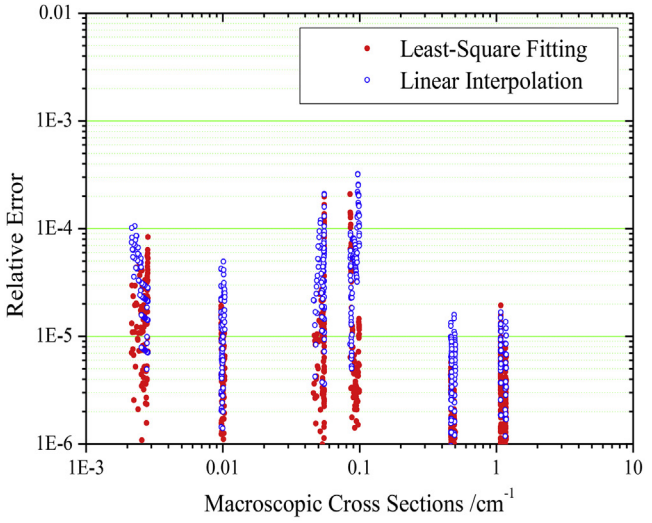


(a) Macroscopic cross sections

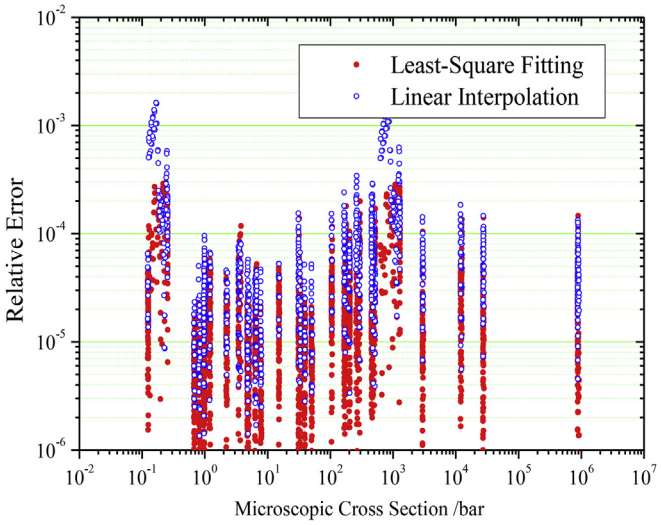


(b) Microscopic cross sections

Fig. 6. Relative error of $f(Bu)$ functionalization for 102 used states out of 196.



(a) Macroscopic cross sections



(b) Microscopic cross sections

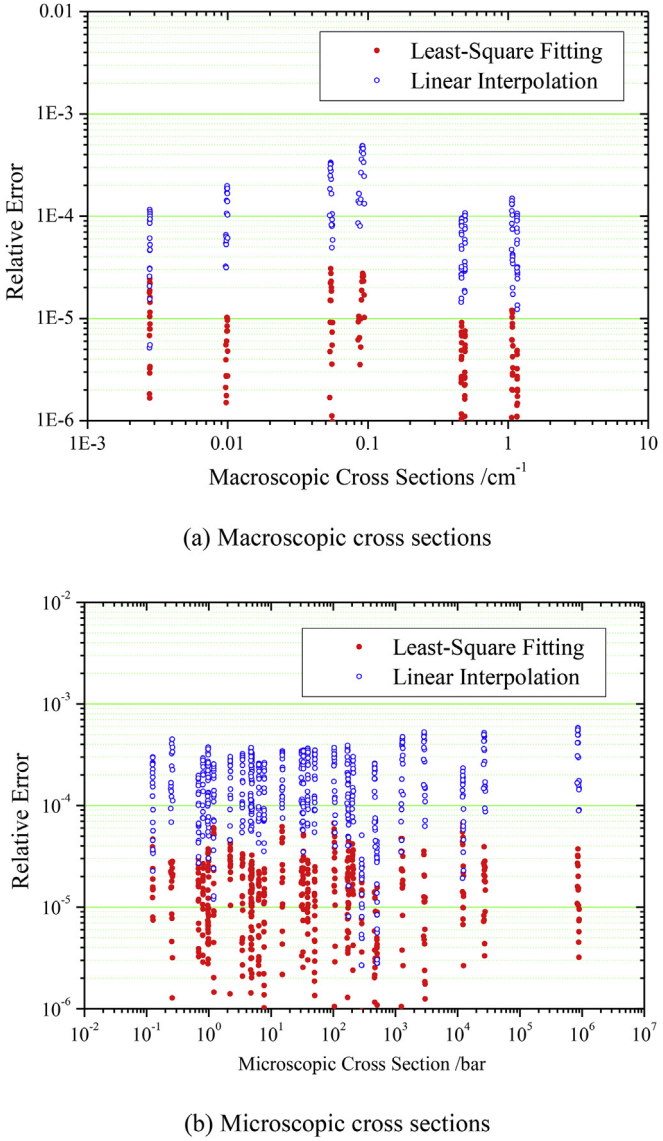
Fig. 7. Relative error of $f(Bu)$ functionalization for 45 used states out of 196.

2.3. History effect treatments

History effect happens mainly due to the fact that *Bu* chosen to indicate the nuclide composition with depletion is a macroscopic parameter. The relationship between *Bu* and the active composition is not a single value reversible relationship. It provides an opportunity for one assembly to reach two states with exactly the same *Bu* but totally different nuclide compositions via two different depletion experiences. For example, two assemblies which are exactly the same at beginning are depleted at two different levels of power and different length of time. As long as the amounts of energy released by them are exactly the same, their *Bu* would be exactly the same. But their nuclide compositions are impossibly to be the same due to the fact that two different depletion calculations (Cacuci, 2011) lying behind. Thus, generally speaking, history effect refers to the difference in few-group constants caused by different depletion conditions such as power level, neutron spectrum and et al.

In order to reduce the history effect as much as possible, the assemblies are traditionally depleted in a most possible condition named as reference condition during the lattice calculation. For other states that do not locate in this depletion line, branch calculation scheme is employed to evaluate the few-group constants. For example, as shown in Fig. 1, the assembly is depleted at $Tf = 923$ K to evaluate the states $\{(Bu, Tf) \mid Bu = 0, 24, 48, \ldots, 120, \ldots$ MWd/tU; $Tf = 923$ K$\}$. For other states such as $\{(Bu, Tf) \mid Bu = 0, 24, 48, \ldots, 120, \ldots$ MWd/tU; $Tf = 723$ K$\}$, their nuclide composition are obtained by switching *Tf* from the corresponding *Bu* states. Those state parameters that can be switched instantaneously during branch calculation have only instantaneous effect the few-group constants, and are named as instantaneous state parameters.

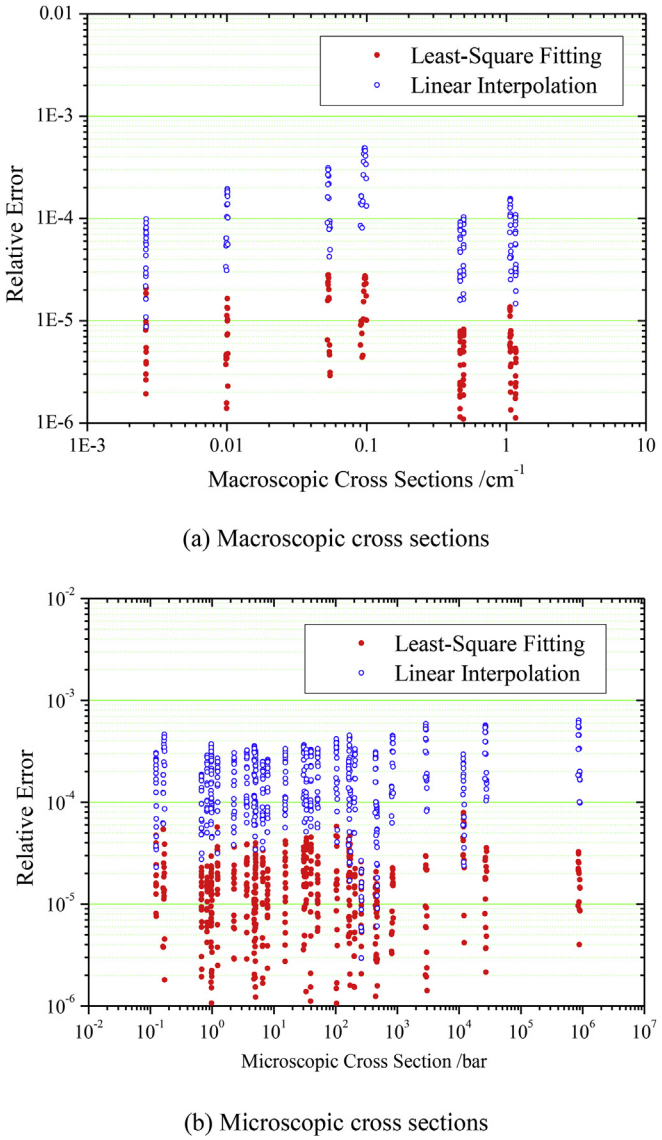
In the code NECP-Lilac, the two widely employed methods have been implemented to treat the history effect, namely the macro-correction method and the micro-depletion method. They are introduced in 2.3.1 and 2.3.2 respectively. In order to make the history effect separated from other approximations within the two-



(a) Macroscopic cross sections

(b) Microscopic cross sections

Fig. 8. Relative error of *f*(*CB*) functionalization for 4 used states out of 21 at 2.0 GWd/tU.



(a) Macroscopic cross sections

(b) Microscopic cross sections

Fig. 9. Relative error of *f*(*CB*) functionalization for 4 used states out of 21 at 10.0 GWd/tU.

step approach, such as the reflective boundary condition during homogenization, an infinite reactor core with the same assembly repeated is selected in this work to compare the two history effect treatments. Thus, the two-group neutron diffusion solution of this core is analytical since there is no leakage any more.

2.3.1. Macro-correction method

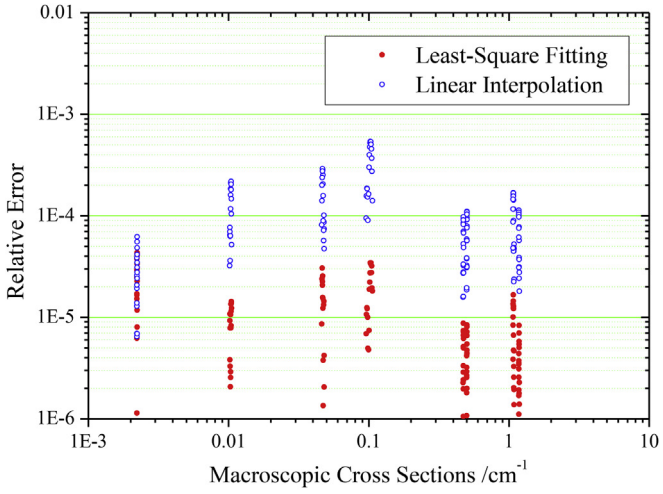
Considering the fact that history effect is caused by different depletion conditions, macro-correction method defines new state parameters to describe the depletion conditions. As long as their contribution to few-group constants can be evaluated, a correction term can be obtained to consider history effect. In contrast to the instantaneous state parameters, these newly defined ones are named history state parameters. Theoretically, each of the instantaneous state parameters can be defined as a corresponding history state parameter.

For instantaneous state parameter V, its history state parameter HV is defined as its weighted average over the past depletion experience:

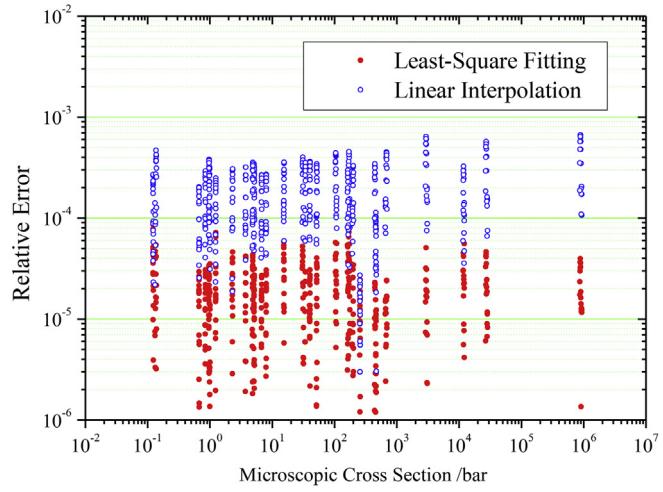
$$HV = \frac{1}{Bu^*}\int_0^{Bu^*} \omega(Bu)V(Bu)\mathrm{d}Bu \tag{14}$$

where Bu^* is the current burnup (MWd/tU), the weighting function $\omega(Bu)$ is experience dependent and usually assumed to be constantly 1.0.

Other than the basic branch calculations, additional depletion calculations have to be carried out to obtain the effect of history state parameters to the few-group constants. Again, take fuel temperature as an example. States $\{(Bu, Tf) \mid 0, 24, 48, \ldots, 120, \ldots$ MWd/tU; $Tf = 723$ K$\}$ are evaluated by direct depletion calculation, similar to the reference ones, as shown in Fig. 2. If the few-group constants at the same states obtained by branch calculation are noted as $\Sigma_{\mathrm{branch}}(V)$, and those obtained by depletion calculation noted as $\Sigma_{\mathrm{depletion}}(V)$, the macro-correction term is defined as:

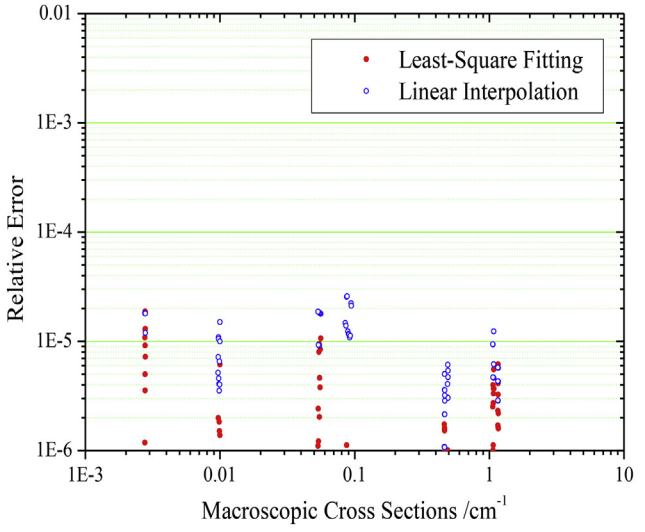


(a) Macroscopic cross sections

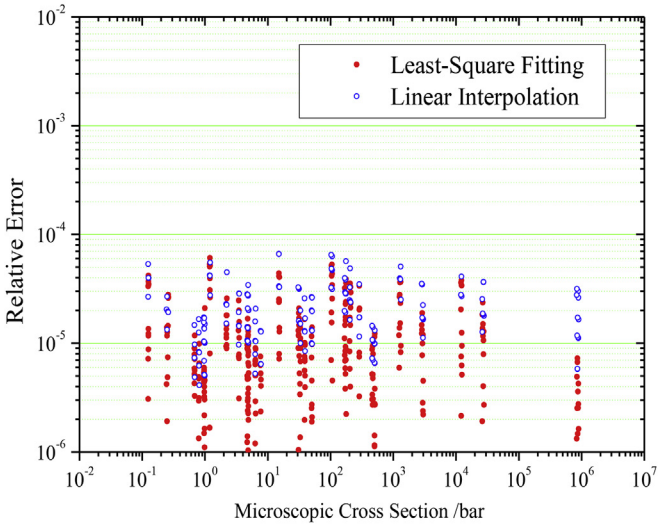


(b) Microscopic cross sections

Fig. 10. Relative error of $f(CB)$ functionalization for 4 used states out of at 30.0 GWd/tU.



(a) Macroscopic cross sections



(b) Microscopic cross sections

Fig. 11. Relative error of $f(CB)$ functionalization for 10 used states out of 21 at 2.0 GWd/tU.

$$\Delta\Sigma(HV) = \Sigma_{\text{depletion}}(V) - \Sigma_{\text{branch}}(V) \tag{15}$$

Thus, the final few-group constants would be the sum of the instantaneous and macro-correction parts.

It can be found that the macro-correction method requires additional lattice evaluations by almost a factor of 2 to obtain the history effects of the few-group constants. Also of course it increases the number of state parameters by almost another factor of 2.

2.3.2. Micro-depletion method

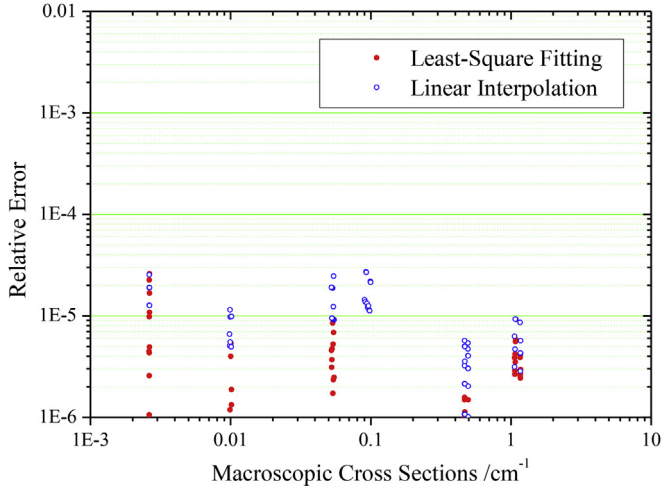
History effect roots in the fact that the macroscopic state parameter *Bu* cannot recognize the single nuclide composition. Thus, the micro-depletion method chooses a number of important nuclides to be tracked online during the core simulation. Once those microscopic cross sections provided to the core simulation, the depletion equation of those nuclides can be solved on-line to track their nuclide densities. And the active macroscopic cross section for neutron diffusion calculation can be assembled back with the history effect considered.

Thus, the few-group macroscopic cross sections are separated into the contributions from the unrecognized and recognized nuclides. The unrecognized ones are still packed together in the form of macroscopic cross sections, while the recognized ones are separated into the multiplication of the corresponding nuclide density and microscopic cross section. Supposing K nuclides are recognized, the few-group constants would be separated:

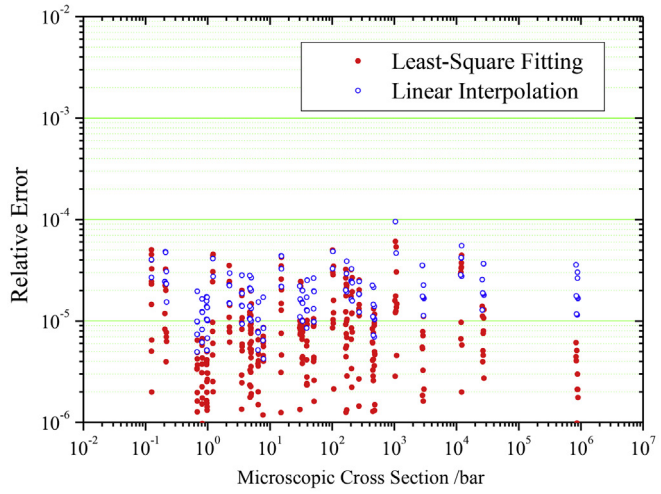
$$\Sigma(\boldsymbol{x}) = \Sigma'(\boldsymbol{x}) + \sum_{k=1}^{K} N^k(\boldsymbol{x}) \cdot \sigma^k(\boldsymbol{x}) \tag{16}$$

where $N^k(\boldsymbol{x})$ and $\sigma^k(\boldsymbol{x})$ are respectively the nuclide density (cm^{-3}) and microscopic cross sections ($\text{cm}^{-2}\ \text{s}^{-1}$) of the kth recognized nuclide obtained from the lattice calculations.

There are two options for how to treat the recognized nuclide densities. (1) The one obtained from the lattice calculation are dropped away, while the one obtain from the on-line depletion calculation are put back to reconstruct the few-group constants. (2) The one obtained from the lattice calculation are also linked. Only

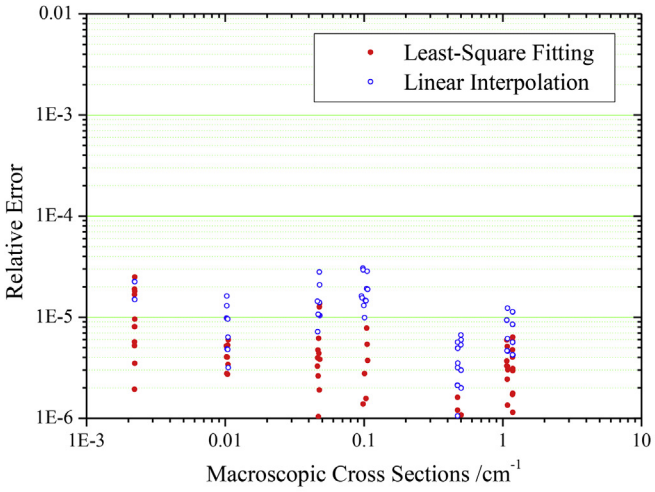


(a) Macroscopic cross sections

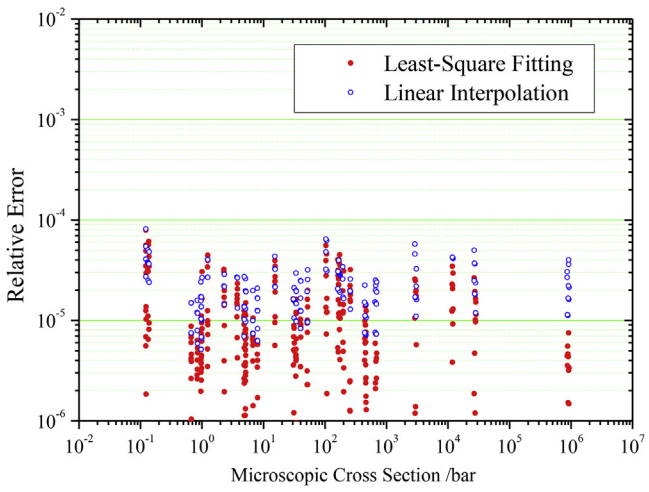


(b) Microscopic cross sections

Fig. 12. Relative error of *f*(*CB*) functionalization for 10 used states out of 21 at 10.0 GWd/tU.



(a) Macroscopic cross sections



(b) Microscopic cross sections

Fig. 13. Relative error of *f*(*CB*) functionalization for 10 used states out of 21 at 30.0 GWd/tU.

the difference between it and the one obtained from on-line depletion are multiplied by the microscopic cross section to take account the history effect. Considering the fact that the difference between these two nuclide density treatments is trivial compared with the difference between micro-depletion and macro-correction methods, only the first one is considered in this paper.

In addition, the on-line depletion calculation during the reactor core simulation would encounter the same situation that the lattice depletion calculation runs in. For the current time step i, the nuclide density, microscopic cross section and neutron flux are all known. To obtain the nuclide density for the next time step $i+1$, the average microscopic cross sections and neutron flux between these two time steps have to be known also, which are unfortunately unknown. Thus, the legacy prediction-correction method for lattice depletion calculation is employed to solve this problem.

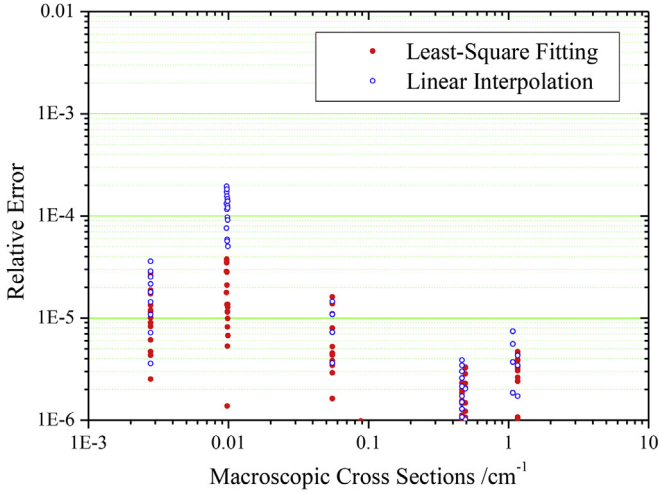
3. Numerical results

In this paper, a typical PWR problem as shown in Fig. 3 is taken as an example to test the theoretical models. All of the materials are the common ones in PWR and can be found in ref. (Gao, 2015), thus omitted here. During the numerical evaluation, the code DRAGON (Marleau et al., 1997) is employed to carry out all the lattice calculations.

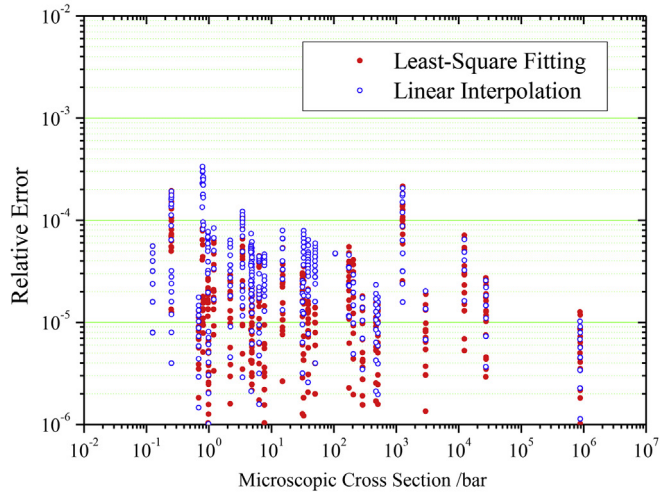
Different from the practical few-group parameterization, more states are evaluated by the lattice code to provide validation reference. The existences of those extra states are ignored during the functionalization and history treatments. In contrast, the state points that are used for functionalization are called used points, while the extra ones just for validation are named raw points.

3.1. The combination of the state parameters

To compare the two combinations in Eq. (1) and Eq. (2) respectively, all the states (4368) shown in Table 1 are evaluated. The corresponding parameterization errors are shown respectively in Fig. 4 and Fig. 5. As in Fig. 4, one can see that even though good precision is observed at used states, errors for raw points are relatively big due to the strong dependence between *CB* and *Tm*. In

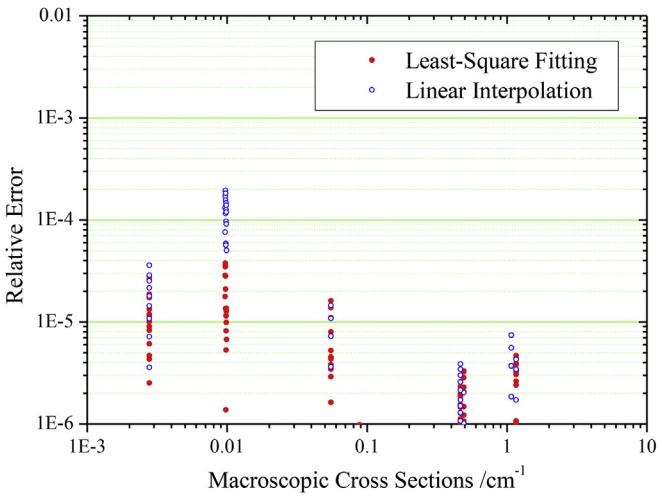


(a) Macroscopic cross sections

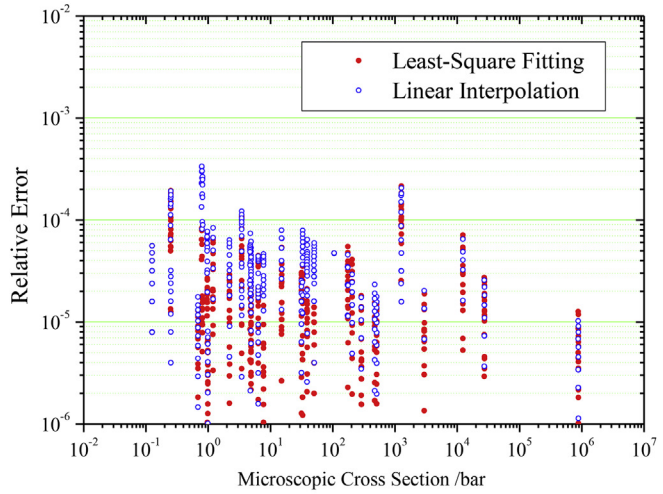


(b) Microscopic cross sections

Fig. 14. Relative error of *f*(*Tf*) functionalization for 4 used states out of 21 at 2.0 GWd/tU.



(a) Macroscopic cross sections



(b) Microscopic cross sections

Fig. 15. Relative error of *f*(*Tf*) functionalization for 4 used states out of 21 at 10.0 GWd/tU.

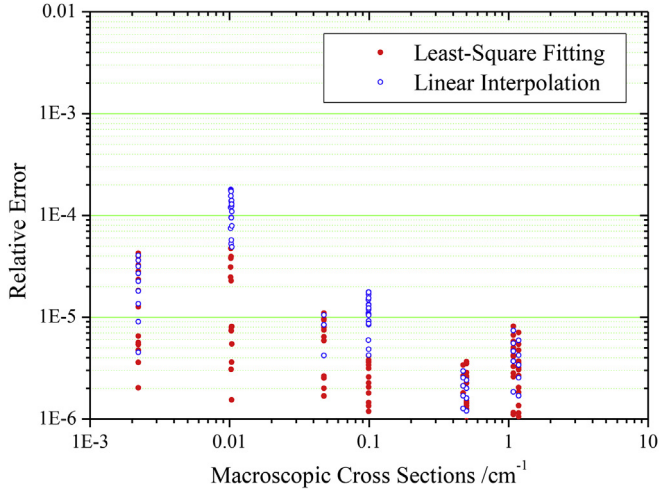
contrast, the maximum error of absorption cross sections (about 1.0% in Fig. 4) is reduced to 0.1% in Fig. 5, and the overall error magnitude is reduced by almost one order of magnitude. Thus the combination of *CB* and *Tm* is suggested for the future PWR few-group constants parameterization.

3.2. Functionalization methods

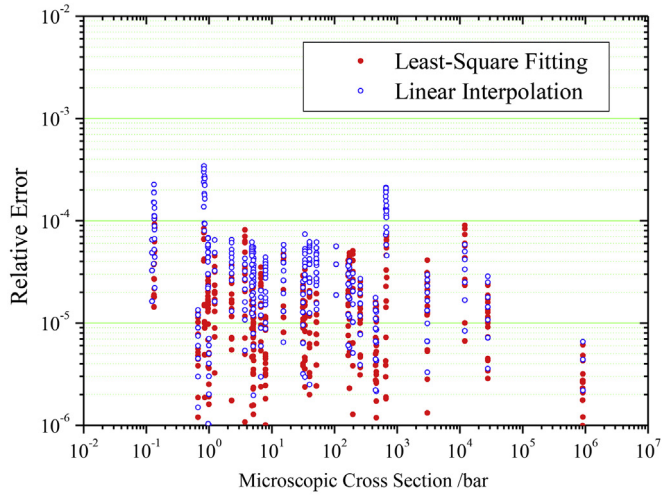
In this subsection, least-square fitting and linear interpolation are compared numerically for each of *Bu*, *CB*, *Tf* and *Tm*. Each of them are evaluated with the others fixed. The few-group constants are macroscopic and microscopic cross sections. Macroscopic ones are the total, fission, absorption and scattering, while microscopic cross sections are the capture (and fission for fissile and fertile) of nuclide ^{235}U, ^{238}U, ^{241}Pu, ^{135}Xe, ^{143}Nd and so on.

For fuel burnup *Bu*, Table 2 lists the 196 states evaluated by the lattice calculation. Two sets of used points are selected. (1) 102 used states including the first 8 and one over two of the rest. (2) 45 used states including the first 8 and one over 5 of the rest. Relative errors of functionalization are summarized in Fig. 6 and Fig. 7. For the least-square fitting method, 45 used state points can provide a maximum error of about 0.02%, while linear interpolation requires 102 used state points to provide a maximum error of about 0.03%. It indicates that linear interpolation requires about two times more state points that the least-square fitting. If only 45 state points are forced to be used by the linear interpolation, the maximum error would be 0.3%, which is one order of magnitude larger than the least-square fitting.

For boron concentration *CB*, lattice calculation evaluated 21 state points for each of the three burnup levels including 2.0 (low), 10 (medium) and 30 (high) GWd/tU at *Tf* = 923.15 K and *Tm* = 583.85 K. These *CB* points are sequentially 0, 100, 200, 300, …, 2000 ppm. Fig. 8, Fig. 9 and Fig. 10 show the relative error of functionalization when 4 states are used. It can be found that the least-square fitting provides a maximum relative error of about 0.01%, while the linear interpolation provides about 0.1%. In contrast, results for 10 used state points are shown in Fig. 11, Fig. 12 and Fig. 13, in which both functionalization methods provide similar precisions with maximum error of about 0.01%.

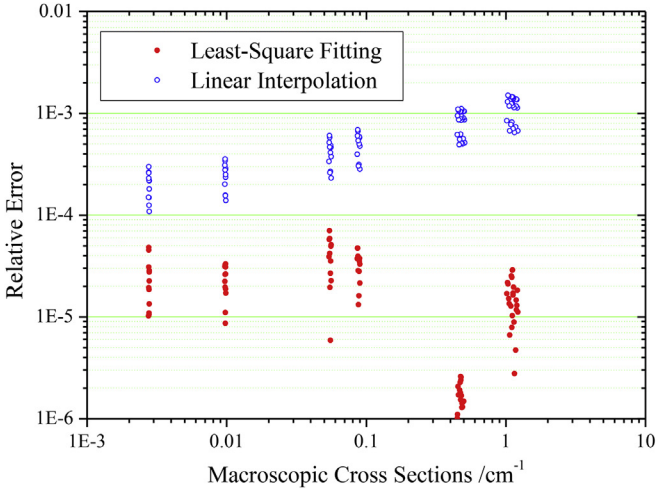


(a) Macroscopic cross sections

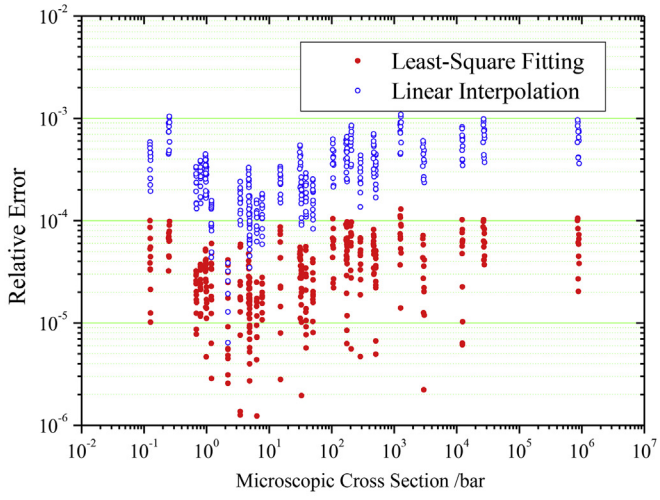


(b) Microscopic cross sections

Fig. 16. Relative error of *f*(*Tf*) functionalization for 4 used states out of 21 at 30.0 GWd/tU.



(a) Macroscopic cross sections



(b) Microscopic cross sections

Fig. 17. Relative error of *f*(*Tm*) functionalization for 4 used states out of 15 at 2.0 GWd/tU.

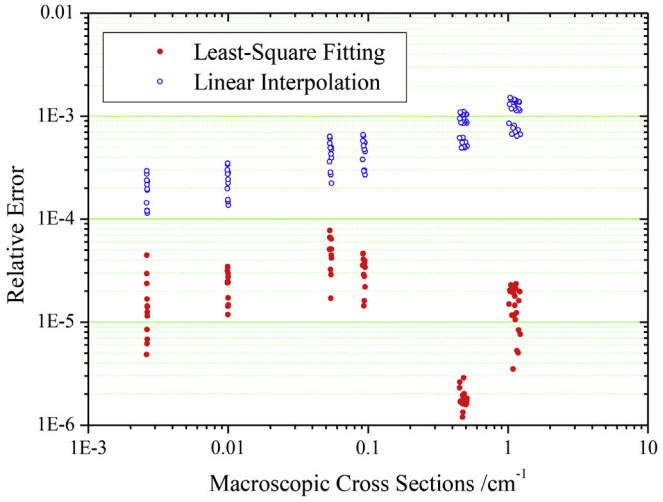
Similarly, also at low (2.0 GWd tU^{-1}), medium (10 GWd tU^{-1}) and high (30 GWd tU^{-1}) levels of burnup, with $Tm = 583.85$ K and $CB = 1000$ ppm, few-group constants are generated at 21 fuel temperatures including 723.15, 743.15, 763.15, …, 1123.15 K. As shown in Fig. 14, Fig. 15 and Fig. 16, however, only 4 used state points are sufficient for both linear interpolation and least-square fitting, simply due to the fact that the function relationship between few-group constants and *Tf* is almost linear in the targeted fuel temperature domain for reactor core simulation.

Moreover, still at the same low, medium and high levels of burnup, with $Tf = 923$ K and $CB = 1000$ ppm, few-group constants are evaluated at 15 moderator temperatures: 566.15, 568.65, 571.15, 573.65, 576.15, 578.65, 581.15, 583.85, 586.15, 588.65, 591.15, 593.65, 596.15, 598.65, 601.55 K. As shown in Fig. 17, Fig. 18 and Fig. 19, functionalization precision of 0.01% can be guaranteed by the least-square fitting even only 4 states (566.15, 583.85, 593.65, 601.55 K) are used. As for linear interpolation, 7 states used (566.15, 571.15, 576.15, 583.85, 588.65, 593.65, 601.55 K) can only reduce the error to be about 0.03%, as shown in Fig. 20, Fig. 21 and Fig. 22.

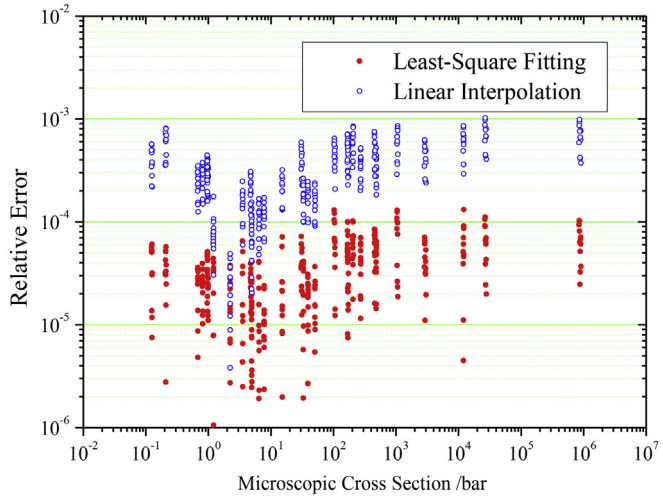
3.3. History effect treatments

It has already been confirmed that both macro-correction and micro-depletion methods provide significant correction effects when the state parameters stay constants along with depletion (Fujita et al., 2014), but not for the histories with state parameters changing during depletion, which happens very frequently in PWR. Thus, this paper selected three typical histories with relative power (as in Fig. 23), boron concentration (as in Fig. 24) and moderator temperature (as in Fig. 25). To keep the depletion chain simplification uninvolved, the micro-depletion chain is exactly the same with the one in the lattice calculation.

Fig. 26 shows the errors of macroscopic cross sections without correction, corrected by the macro-correction method and corrected by the micro-depletion method for the relative power history, while Fig. 27 and Fig. 28 are respectively for the *CB* and *Tm* histories. For the power history, both micro-depletion and macro-correction methods provide correction effects. But the contribution of micro-depletion is more visible. However, for boron

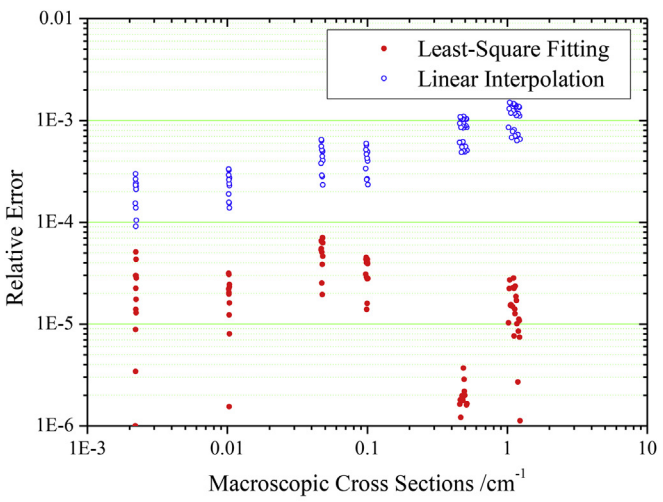


(a) Macroscopic cross sections

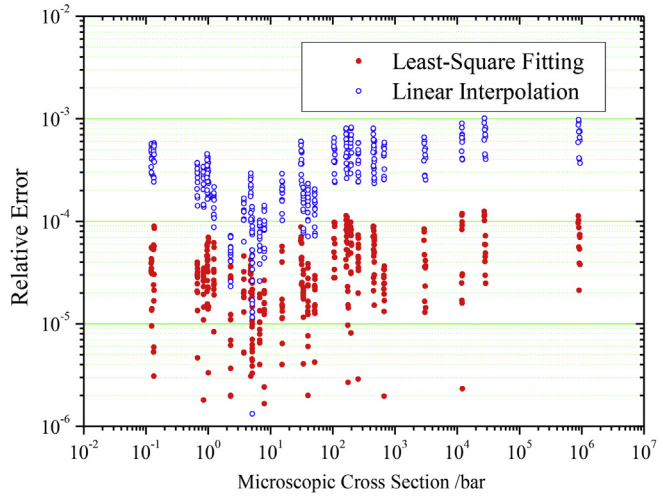


(b) Microscopic cross sections

Fig. 18. Relative error of *f*(*Tm*) functionalization for 4 used states out of 15 at 10.0 GWd/tU.

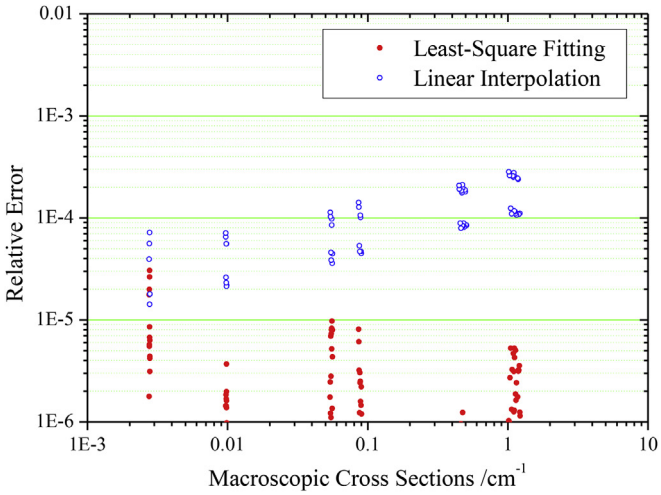


(a) Macroscopic cross sections

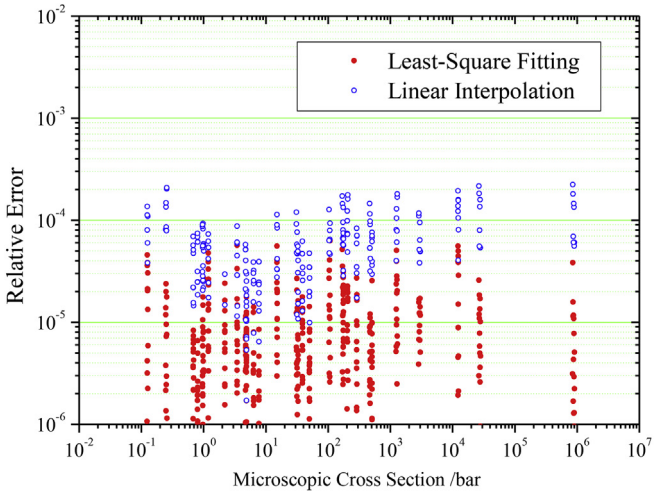


(b) Microscopic cross sections

Fig. 19. Relative error of *f*(*Tm*) functionalization for 4 used states out of 15 at 30.0 GWd/tU.

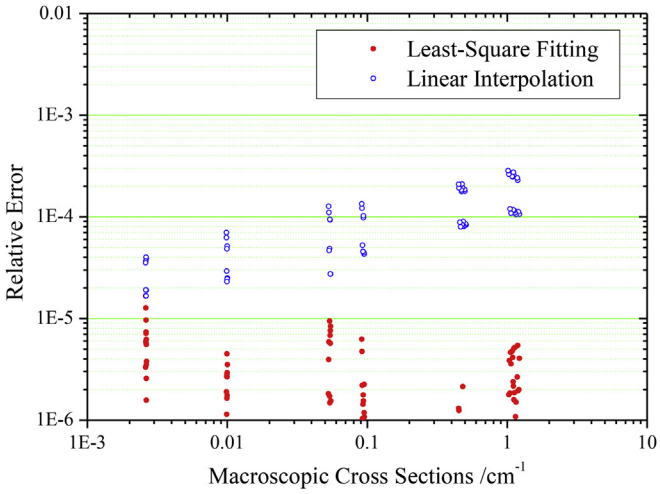


(a) Macroscopic cross sections

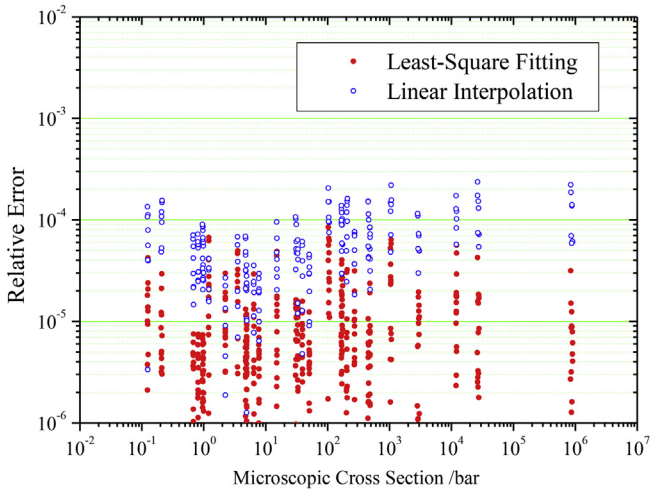


(b) Microscopic cross sections

Fig. 20. Relative error of *f*(*Tm*) functionalization for 7 used states out of 15 at 2.0 GWd/tU.



(a) Macroscopic cross sections



(b) Microscopic cross sections

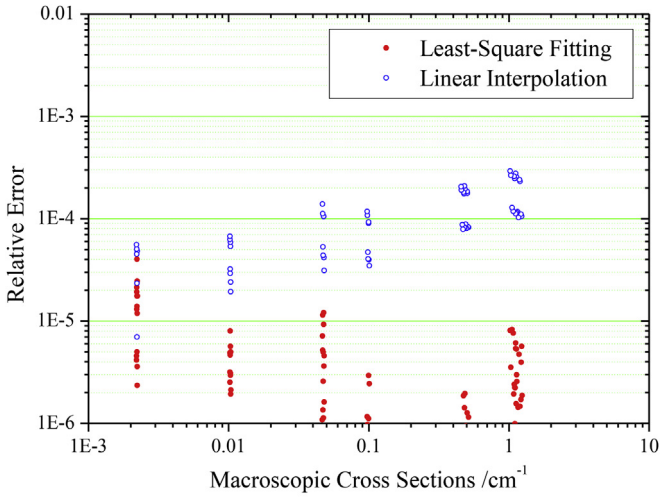
Fig. 21. Relative error of *f*(*Tm*) functionalization for 7 used states out of 15 at 10.0 GWd/tU.

concentration history and moderator temperature histories, the macro-depletion method appears to increase the error instead of reducing it.

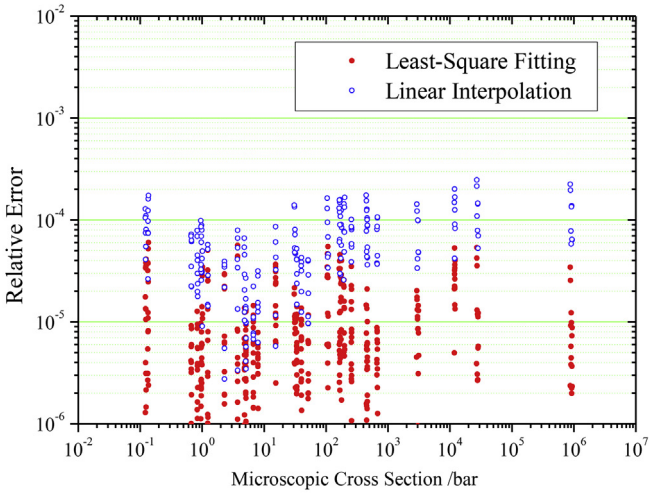
However, what must be mentioned is that the micro-depletion method demands depletion calculation in reactor core simulation which can be time and memory consuming. In addition, it is obvious that the error after micro-depletion method applied is still not zero. This is mainly due to the spatially homogenized an energy group condensed microscopic cross sections of the recognized nuclides. They are also affected by the depletion history through the heterogeneous flux spectrum in space and energy group, but remain uncorrected in this paper.

4. Conclusions

PWR few-group constants parameterization is investigated by developing a general code named NECP-Lilac. There are three main aspects summarized in this paper, which are the combination of state parameters, functionalization methods and the history effect treatments. (1) As for the combination of state parameters, other than combining (*Bu*, *CB*) and (*Bu*, *Tm*) separately, the combination of (*Bu*, *CB*, *Tm*) is suggested to take account the coupling effect of boron concentration and moderator temperature, which would reduce the parameterization error by almost one order of magnitude. (2) Other than the logical knowledge that linear interpolation requires more state points to get a similar precision with the least-square fitting, it has been found numerically that the corresponding factor is about two for almost each state parameter which means that linear interpolation requires more than one order of magnitude lattice calculations than the least-square fitting method. However, the choice of fitting order and segment division is very experience-dependent. Thus, the linear interpolation is recommended for new reactors or other applications, while the least-square fitting is more feasible for routine calculation in engineering applications. And the code NECP-Lilac can be employed to obtain the experience on the selection of polynomial order and the segmentation. (3) For the macro-correction and micro-depletion methods, it has been found that in cases where state parameter varies along with depletion, the micro-depletion method can always reduce the error by half or even an order of magnitude, while



(a) Macroscopic cross sections



(b) Microscopic cross sections

Fig. 22. Relative error of $f(Tm)$ functionalization for 7 used states out of 15 at 30.0 GWd/tU.

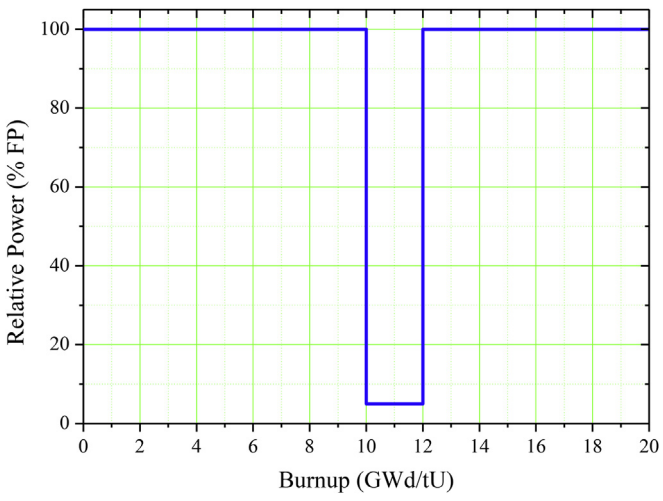


Fig. 23. Relative Power history.

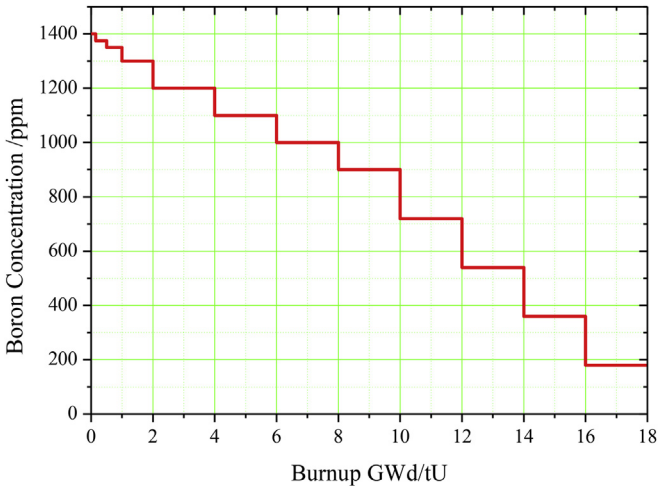


Fig. 24. Boron concentration history.

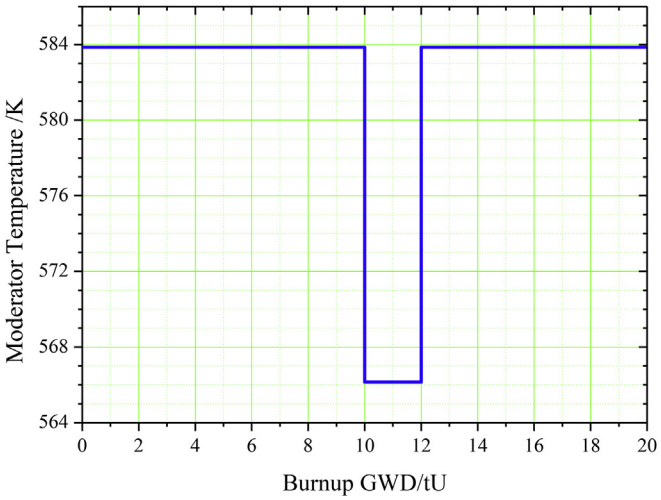


Fig. 25. Moderator temperature history.

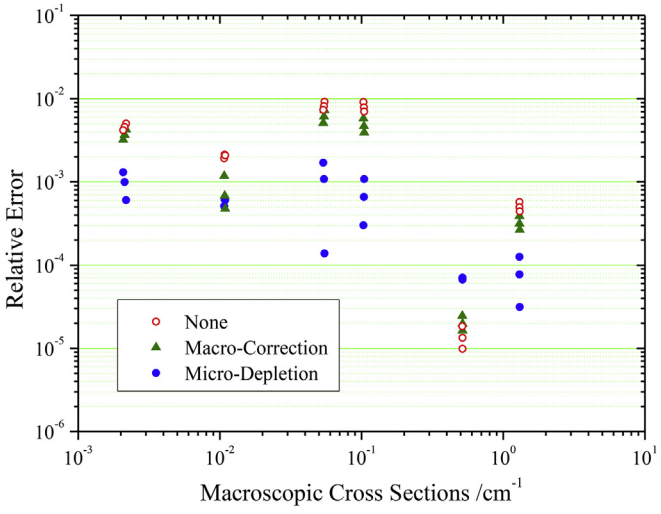


Fig. 26. Correction for relative power history.

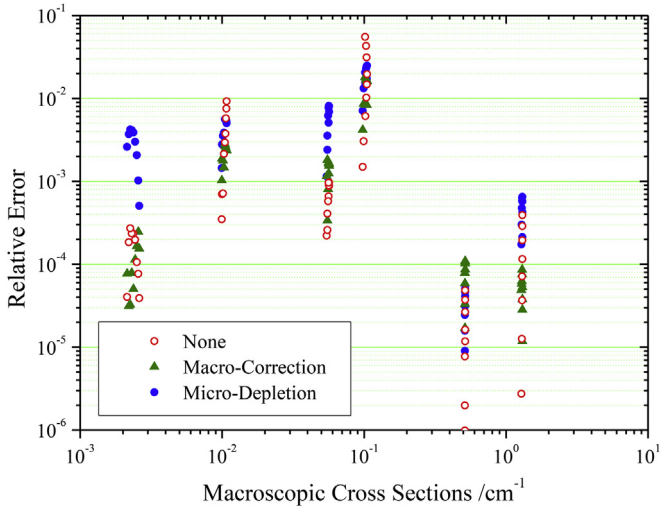


Fig. 27. Correction for boron concentration history.

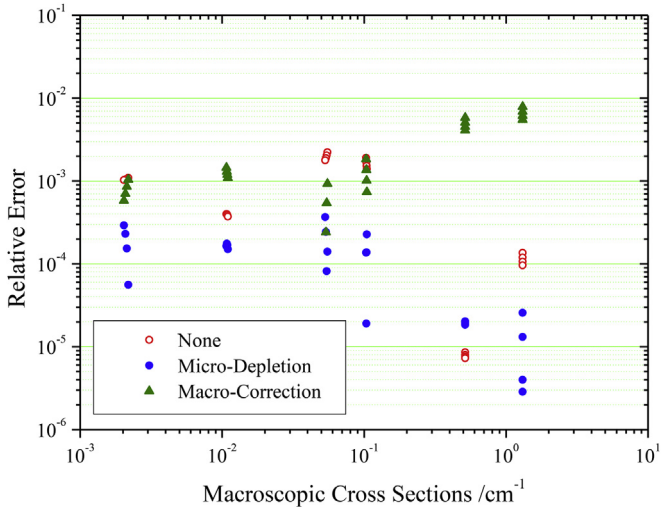


Fig. 28. Correction for fuel temperature history.

the macro-correction method may introduce error instead of reducing it.

However, there are still topics left for future investigation. (1) It is the simplification of the depletion chain. (2) It is the correction of microscopic cross sections.

Acknowledgment

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