### Comparison of Cross-Section Models for Functionalization and History Effect

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# INTRODUCTION

Considering time and storage consumptions, nuclear reactor physics calculation is usually approximated into two steps, namely the lattice and core calculations. The former provides lattice homogenized few-group cross sections for discretized state variables such as burnup, fuel temperature, moderate temperature and density, boron concentration and et al. The later core calculation simulates the actual core performance by using these few-group cross sections. Unavoidably, the actual lattice state usually is not one of the states provided by the lattice calculation, requiring a continuous relationship between these few-group cross sections and state variables. This functionalization is usually performed by a link code between the lattice and core calculations. Meanwhile, the actual depletion history of the lattice in the core is unavoidably different from the one in the forgoing lattice simulation. It makes the actual fewgroup cross sections practically required by the core calculation different from the ones obtained after the link process even they have exactly the same state variables. This is called history effect<sup>[1]</sup>, which is usually also expected to be handled during the link process. Both the lattice and core calculation processes themselves can provide accurate results as long as their inputs are sufficiently accurate. It turns out to be the link process that introduces the most of the errors during nuclear reactor physics simulation. Thus, a general link code named NECP-LILAC has been developed to investigate cross section models of functionalization and history effect.

Numerous methods exist today in different simulation codes, of which linear interpolation<sup>[2]</sup> and least-square interpolation<sup>[3]</sup> are the most widely used ones. Meanwhile, history effect becomes more and more important as simulation becomes more and more accurate, leading the development of various correction methods including macro-correction<sup>[4]</sup> and micro-depletion<sup>[4]</sup> methods. Unfortunately, there is still no clear suggestion on how to choose a cross-section model for a specific problem. Thus, this summary compares the linear interpolation and least-square interpolation for cross section functionalization, macro-correction and micro-depletion for history effect correction.

#### FUNCTIONALIZATION METHODS

As only cross-sections at a limited number of states are calculated with lattice code, actual cross-sections required by core simulation must be obtained with a certain function determined by the lattice-code-given cross-section library. Linear interpolation only takes cross-sections at the two calculated states the most close to the unknown one for each state parameter and gets a linear approximation of the crosssections needed. In contrast, least-square interpolation can give the function with a minimum total error of all state points used for functionalization.

Obviously, least-square interpolation has the advantage of representing cross-sections with high order polynomials. In cases where the dependence of cross-section values on a considered state parameter tends to be, for example, a quadric or cubic curve, it can be very easy to get a highly precise approximation with least-square interpolation. On the contrary, when it comes to linear interpolation, a lot more state points are required to well reproduce the crosssection tendency, which means a lot more lattice code calculation should be performed.

In addition, what should be mentioned for least-square interpolation is that analysis has to be done in advance on the cross-section tendency so as to be conscious of polynomial orders to choose. Moreover, for state parameters of which the change of value is significant, such as burnup, the entire range must be divided to several segments and least square interpolation must be done in each to avoid oscillations. In comparison, linear interpolation requires none of these procedures described and as long as enough state points are provided good precision can be achieved, which is very practical.

Comparisons are made with the self-developed crosssection modeling code NECP-Lilac, which can produce either linear interpolation or least-square interpolation. A typical  $17 \times 17$  PWR assembly was calculated at different burnup steps. For each burnup step, 21 boron concentrations (*CB*) are simulated as listed in Table I. Functionalization of macroscopic cross section and boron concentration were carried out for each burnup step to compare the two methods. In case 1, only 4 *CB* points as listed in Table I were used as known states, while the rest 17 points employed as verification data. In Case 2, 10 knowns and 11 verifications also as listed in Table I. Fig. 1 and Fig. 2 show the relationship between the relative error of cross section and the value of these cross sections, respectively for Cases 1 and 2.

From Fig. 1, we can find that with the same number of states used for functionalization which is very few, least-square interpolation is more precise. From Fig. 2, we can find that with the number of states used for functionalization increased, linear interpolation can achieve a similar

accuracy with least-square interpolation. When looking at the 2 cases together, the precision of least square interpolation barely changes with more functionalization states used. Consequently, conclusion can be drawn that in this problem with only 4 states one can get a good precision with the maximum relative error of 1pcm using least-square interpolation while 10 would be required by linear interpolation. Thus, it is roughly about 2 times.

Table I Boron Concentrations (CB)

	Boron concentrations (ppm)
Lattice Calculation	0, 100, 200, 300, 400, 500, 600, 700, 800, 900, 1000, 1100, 1200, 1300, 1400, 1500, 1600, 1700, 1800, 1900, 2000
Functionalization Case 1	0, 500, 1000, 2000
Functionalization Case 2	0, 200, 400, 800, 1000, 1200, 1400, 1600, 1800, 2000

### HISTORY EFFECT CORRECTION METHODS

History effect refers to the difference of cross-sections observed between those pre-calculated using lattice code and the real ones needed at the same macroscopic state points during core simulation. Here macroscopic state point means the same state variables such as burnup, fuel temperature, moderator temperature, boron concentration, and et al. The reason is that a lattice may experience different histories to reach the same state point, which means these macroscopic state variables can only take in account the instantaneous effect, not the corresponding nuclide density change process<sup>[1]</sup>.

The macro-correction method<sup>[4]</sup> adds a new state variable to refer the history of each macroscopic state variable except burnup (Bu). For macroscopic state variable V, it history state variable is defined as:

$$HV = \frac{1}{Bu^*} \int_0^{Bu^*} \omega(Bu) \cdot V(Bu) dBu$$
(1)

where  $Bu^*$  stands for the current burnup, V(Bu) refers to the actual history of V vs Bu, and  $\omega(Bu)$  is a weighting function considering different part of history contributes differently.

Correspondingly, a cross section history correction can be defined as:

$$\Delta \Sigma(HV) = \Sigma(V_{dep}) - \Sigma(V_{ref})$$
<sup>(2)</sup>

where  $\Sigma(V_{\text{ref}})$  and  $\Sigma(V_{\text{dep}})$  correspondingly refers to the cross section obtained after a reference and actual depletion history. By functionalization of this cross section correction to modify the core cross sections, history effect can be considered.

## Reactor Analysis Methods-I

In contrast, the micro-depletion method functionalizes microscopic cross sections for selected nuclides and solves their depletion equation during core simulation to capture their nuclide density change process.

It is shown that both of the above two methods work very well when correcting a history with the state parameter fixed at known value for one history<sup>[1,4]</sup>. However, during core simulation one is often confronted with such histories in which state parameters change during depletion. Fig. 3 shows a typical power change process one could observe in BEAVRS (Benchmark for Evaluation And Validation of Reactor Simulations) first cycle<sup>[5]</sup>. It drops from 100% to nearly 0% at Bu=10GW/tU and then goes back up to 100% at Bu=12GW/tU.

Both of the above methods were employed to consider the process shown in Fig. 3. Taking the active history process as refference, relative error of cross sections recovered by both methods are shown in Fig. 4. One can find that in this case, macro-correction method makes a very small difference compared to cross-sections without considering history effect, while micro-depletion method reduces relative error from about 1.0% to 0.1%.

On one hand, why the micro-depletion method works better than macro-correction method? The main reason is that the relationship between depletion history and history variable HV is not a single-value map. A single variable cannot represent a fixed depletion process. On the other hand, why the micro-depletion method cannot eliminate all the error? That is mainly because of the microscopic cross sections. During lattice calculation, spatial homogenization and energy group condensation were done, making the microscopic cross sections of different nuclides affect each other through flux spectrum. Even if the micro-depletion method can capture exactly all the nuclide densities, without exact microscopic cross sections, error would be introduced into the macroscopic cross sections. What actually happens is that nuclide densities cannot be exactly track down without exact microscopic cross sections.

## CONCLUSIONS

Two widely used functionalization methods, least square interpolation and linear interpolation, and two wellknown history effect correction methods, macro-correction method and micro-depletion method, have been compared in this work.

For functionalization, least-square interpolation can limit the number of states needed and thus demands fewer lattice calculations. But it requires experience to determine the state variable sub-segments and the expansion orders.. In contrast, linear interpolation requires more lattice calculations but can treat more common problems without any experience. Next, more effort is going to put at the segment and expansion order selections in least-square interpolation for specific problems. Reactor Analysis Methods-I



Fig. 1 Cross-section relative error in Case 1

Fig. 2 Cross-section relative rrrors in Case 2

For history effect correction, both macro-correction method and micro-depletion method work in case of state parameter changing during depletion, but micro-depletion method has a more significant effect. More study is required for how to consider history effect in microscopic cross sections.



Fig. 3 Power change in depletion process



Fig. 4 Relative error of cross-sections for history effect

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