GENERALIZED DEPLETION CHAIN SIMPLIFICATION BASED ON SIGNIFICANCE ANALYSIS

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ABSTRACT

The depletion chain defined by evaluated nuclear data library is unnecessarily complex for most applications in reactor physics. The simplification methods are confronted with two difficulties. Firstly, the number of possible simplified depletion chains is excessively large. Secondly, depletion calculation is dynamic process coupled with neutronics, which means the simplified depletion chain has to be able to catch the main features of the entire physical process. Thus, in this paper, a generalized depletion chain simplification method is proposed with limited approximations employed. It defines the significance of the entire depletion calculation as the neutron production and absorption and the number densities of the important nuclides. And then it evaluates the significance value of each reaction channel and decay nuclides by perturbed depletion calculations. Since short-lived nuclides are intended to be reduced from the depletion chain, delayed decay heat precursors are introduced in order to consider short-term decay heat.

Key Words: **Depletion chain simplification, Significance value, Decay heat precursor**

1. INTRODUCTION

The composition evolution of nuclear fuel is an important issue of reactor physics. The set of considered nuclides and transfer relations (decay or neutron-induced) among them, which are referred to as depletion chain, constitute the foundation of problem simulation effort. The depletion chain stored in the evaluated nuclear data library contains thousands of nuclides and much more number of transfer relations. This complex depletion chain is not necessary, if not practical, for most reactor physics applications. Since most of the transfer relations are not responsible for transformation of significant amount of nuclide number density, and most of the nuclides decay rapidly enough for reaching secular equilibrium. Depletion chain simplification methods deal with projection of the complex original depletion chain to simpler depletion chain. With prescribed complexity level and the accuracy requirements, the simplified chain produced by an ideal method should be superior in a sense that the nonexistence of a simpler and more accurate chain is guaranteed. However, the possibilities of the simplified chain are prohibitively large in number, and the application conditions (such as geometry, initial composition and power history) are also changeful. It is therefore difficult to find an ideal method of practical computational cost, and the proposed methods all require some specific approximations.

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The method used in WIMS-D Library Update Project (WLUP) is semiempirical [1], it employs a set of quantitative criteria to select nuclides. The Contribution Matrix method utilizes powers of defined contribution matrix to identify nuclides that have significant influences on target nuclides [2], each element of contribution matrix represents the ratio of inter-nuclide production rate to total production rate. The Singular Value Decomposition (SVD) method uses row-normalized depletion matrix and SVD of matrices to find out nuclides that are important for target nuclides production [3], each element of row-normalized depletion matrix is no greater than 1.0. The adjoint calculation method finds the nuclides that the derivatives of target nuclides number densities in the last depletion step with respect to initial number densities of such nuclides are greater than defined criteria [4]. The WLUP method maintains the neutronic calculation accuracy excellently, while it could not deal with the accuracy requirement of target nuclides number densities. The Contribution Matrix method and SVD method ignore the absolute reaction rates, which is a large approximation. The adjoint calculation method focuses on the significance analysis of nuclides number densities, it makes use of perturbation theory and depends on less approximation. However, the method could not give out complete instructions for the simplification process, because the adjoint calculations are based on original depletion chain and the effects of a modification in the chain (such as setting a decay nuclide in secular equilibrium state) could not be evaluated by this method.

This paper is organized as following. Section 2 focuses on definition of accuracy degradation due to a modification in the depletion chain, or the significance value of the modification. Section 3 is responsible for detailed description of the simplification method. Section 4 gives numerical results of a PWR pin cell problem. Finally, conclusions are drawn in section 5.

2. DEFINITION OF SIGNIFICANCE VALUE

Different applications have varying problem definition domains and accuracy requirements. The problem definition domain is represented by a typical pin cell problem in this study. The following analysis is based on a depletion calculation of the representative pin cell problem, and the number of depletion steps is *I*.

The accuracy requirements include neutronic aspects, radioactivity, toxicity, etc. The neutronic aspects will be discussed explicitly, while the other requirements will be converted to number densities of target nuclides, which have important contributions to specific requirements.

2.1. Neutronic Aspects

The considered neutronic aspects include the neutron fission production and the neutron absorption loss.

2.1.1. Neutron production by fission

In the *i'th* depletion step, the total neutron production by fission in unit volume is expressed as:

$$\Omega_{i,\text{fission}} = \phi_i \sum_{\substack{j=1 \\ j\in \mathbf{HM}}}^{n} \overline{N}_{i,j} \sigma_{i,j,\text{f}} \mu_{i,j} t_i \tag{1}$$

where ϕ_i is the neutron flux, **HM** is the set of heavy metal nuclides, *n* is the number of nuclides, $\overline{N}_{i,j}$ is the average number density of *j'th* nuclide, $\sigma_{i,j,\mathrm{f}}$ is the fission cross section of *j'th* nuclide, $\mu_{i,j}$ is the average neutron emission per fission of *j'th* nuclide, t_i is the depletion time.

2.1.2. Neutron loss by absorption

In the *i'th* depletion step, the total neutron loss by absorption in unit volume is as follows:

$$\Omega_{i,\mathrm{absorption}} = \phi_i \sum_{j=1}^{n} \overline{N}_{i,j} \sigma_{i,j,\mathrm{a}} t_i \tag{2}$$

where $\sigma_{i,j,\mathrm{a}}$ is the absorption cross section of *j'th* nuclide.

2.2. Number Densities of Target Nuclides

The target nuclides are identified from their contributions to specific accuracy requirements as mentioned above, and they constitute the nuclide set **T**. The number density of *j'th* nuclide at the end of *i'th* depletion step is denoted as $N_{i,j}$.

2.3. Significance Value of a Modification

For a modification of depletion chain, e.g. deleting a reaction channel, its significance value pair is defined in Eqn. (3).

$$\begin{aligned} L_a &= \max\left\{1 \le i \le I \mid w_{\mathrm{f},i} \frac{\left|\Omega'_{i,\mathrm{fission}} - \Omega_{i,\mathrm{fission}}\right|}{\Omega_{i,\mathrm{fission}}}\right\} + \max\left\{1 \le i \le I \mid w_{\mathrm{a},i} \frac{\left|\Omega'_{i,\mathrm{absorption}} - \Omega_{i,\mathrm{absorption}}\right|}{\Omega_{i,\mathrm{absorption}}}\right\} \\ L_b &= \max\left\{1 \le i \le I \mid w_{\mathrm{n},i} \sum_{\substack{j=1 \\ j \in \mathrm{T}}}^{n} w_{\mathrm{nuclide},j} \frac{\left|N'_{i,j} - N_{i,j}\right|}{N_{i,j}}\right\} \end{aligned} \tag{3}$$

where the prime symbol indicate after modification values, $w_{\mathrm{p},i}$, $w_{\mathrm{a},i}$, $w_{\mathrm{n},i}$ and $w_{\mathrm{nuclide},i}$ are the weighting factors.

3. PROCESS OF THE SIMPLIFICATION METHOD

3.1. Representative Neutronic-depletion Coupled Calculation

The reference cross sections, neutron flux and nuclide number densities employed in the analysis come from neutronic-depletion coupled calculation of a representative pin cell problem. The neutronic part is OpenMC [5], while the depletion part and coupling scheme is home-made.

3.2. Significance Value of Reaction Channels

For each decay channel or neutron reaction channel, the after modification nuclide number densities and time-averaged number densities is calculated by direct perturbed depletion calculation. The transfer coefficient of corresponding channel is set to be zero in the perturbed calculation. Then significance value pair is found by substituting after modification nuclide number densities and time-averaged number densities in Eqn. (3).

3.3. Significance Value of Decay Nuclides

The depletion chain can also be simplified by reducing decay nuclides. A decay nuclide is called to be reduced, if all transfer relations that reach this nuclide are modified to reach its decay daughters directly, this treatment is equivalent to setting the decay nuclide in secular equilibrium state.

If a nuclide's decay constant is lower than λ_1 (the decay half-life should be comparable to fuel cycle length), then its significance value pair is given a high enough value to prevent it from being reduced. On the other hand, if a nuclide's decay constant is higher than λ_2 (large value to ensure the dominating role of decay in its transfer process), then its significance value pair is set to be zero. For those decay nuclides that have their decay constants between λ_1 and λ_2, the after modification (which is the reduction of the decay nuclide) number densities and averaged number densities are obtained by setting the decay constants being λ_2. Then the significance value pair is calculated by Eqn. (3).

3.4. Modification Processes

A nuclide or reaction channel is identified as non-significant, if both elements of its significance value pair are lower than corresponding preset criteria $svcut_1$ and $svcut_2$, otherwise it is identified as significant. The simplified depletion chain is obtained through the following processes:

1) Mark the non-significant reaction channels and decay nuclides;
2) For those decay nuclides that are marked and do not have unmarked reaction channels, they are reduced from the depletion chain;
3) For those nuclides that do not have unmarked reaction channels, and its contribution fractions to neutron production and neutron loss are both lower than $svcut_1$, they are deleted.

4. NUMERICAL RESULTS

The reference depletion chain is based on ENDF/B-VII.0. The data source includes decay library, neutron-induced fission product yield library, and neutron reaction channels with representative single group cross sections (neutron reaction channels with cross sections lower than 1 mbarn are neglected) generated by PREPRO [7]. Then the depletion chain is further simplified by confining neutron channels to radioactive capture, fission and (n,2n). Finally the reference depletion chain is obtained by excluding nuclides that cannot be generated from ^{235}U, ^{238}U or ^{16}O.

The representative pin cell problem is the UO_2 fuel pin from a burnup benchmark suite [8]. The problem specification is summarized in **Table 1**.

Table 1. Pin cell problem specification

	UO_2 fuel pin
Fuel rod pitch	1.265 cm
Pellet outer diameter	0.824 cm
Cladding inner diameter	0.824 cm
Cladding outer diameter	0.952 cm
^{235}U enrichment	6.5 wt%
UO_2 density	10.3 g/cc
Fuel region composition (#/(barn · cm))	Temperature : 900K
^{235}U	1.5122E-03
^{238}U	2.1477E-02
^{16}O	4.5945E-02
Cladding composition (#/(barn · cm))	Temperature : 600K
Zr-nat.	4.3107E-02
Coolant composition (#/(barn · cm))	Temperature : 600K
H_2O	2.2074E-02

The parameters used in simplification process are chosen as follows: $w_{\mathrm{p},i}$, $w_{\mathrm{a},i}$, $w_{\mathrm{n},i}$ are set to be $\delta_{i,4} + \delta_{i,15} + \delta_{i,25} + \delta_{i,37}$, corresponding burnup values for these steps are 1, 10, 40 and 70 (unit : GWd/tHM) respectively; $w_{\mathrm{nuclide},i}$ equals to 1.0 for all nuclides and all steps; λ_1 and λ_2 are set to be 1.0E-7 and 1.0 (unit : s^{-1}) respectively. And 35 target nuclides are selected: Mo-95, Tc-99, Ru-101, Rh-103, Rh-105, Pd-105, Pd-107, Pd-108, Ag-109, I-135, Xe-131, Xe-135, Cs-133, Cs-134, Nd-143, Nd-145, Pr-141, Pm-147, Pm-148, Pm-148m, Pm-149, Sm-147, Sm-149, Sm-150, Sm-151, Sm-152, Eu-153, Eu-154, Eu-155, Gd-154, Gd-155, Gd-156, Gd-157, U-239, Np-239. The main characteristics of reference and simplified chains are listed in **Table 2**.

Table 2. Main characteristics of depletion chains

Chain name	$svcut_1$	$svcut_2$	Number of nuclides	Number of fission products
Reference	---	---	1304	1137
Chain-1614	1.0E-6	1.0E-4	185	155
Chain-1612	1.0E-6	1.0E-2	178	148
Chain-1514	1.0E-5	1.0E-4	149	122
Chain-1512	1.0E-5	1.0E-2	132	105

The k-infinity results of different depletion chain calculations are shown in **Fig. 1**. k-infinity errors compared with reference chain calculation are provided in **Fig. 2**.

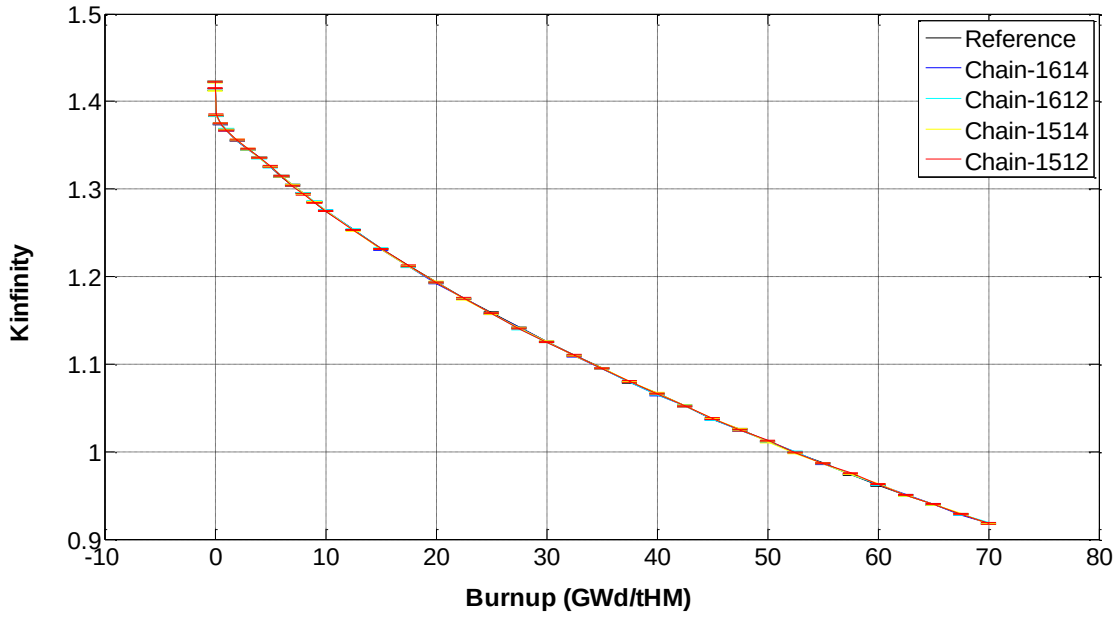

Fig 1. K-infinity results of different depletion chains

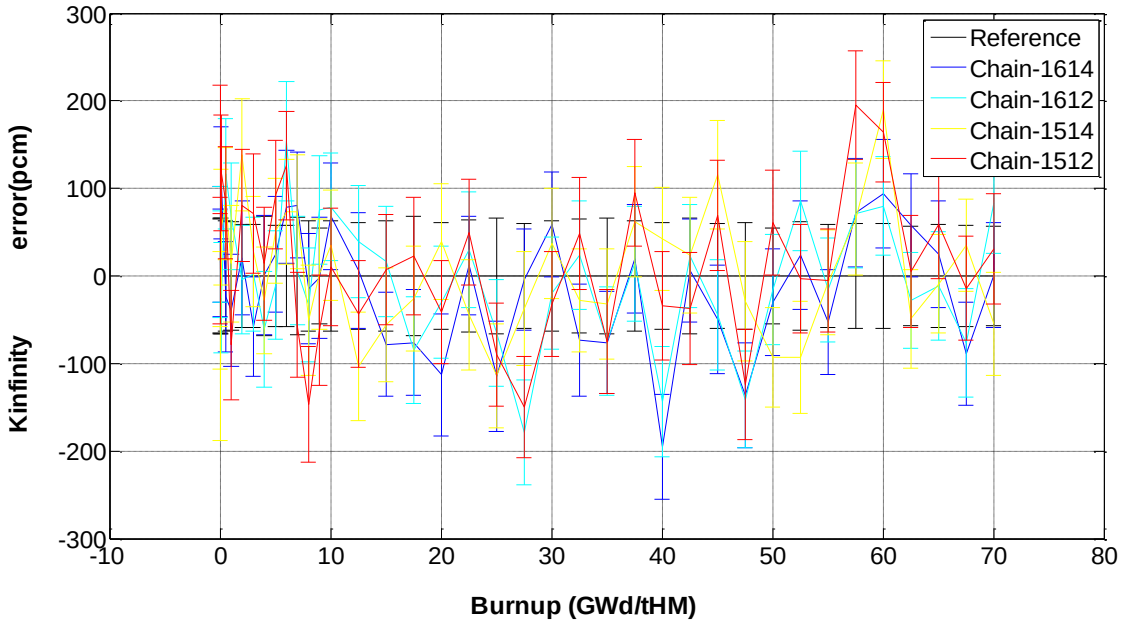

Fig 2. K-infinity errors compared with reference chain (pcm)

The neutronic calculation is performed with 60 inactive batches and 200 active batches, each batch contains 10000 neutrons, and the stochastic errors estimated by OpenMC are plotted as vertical bars in the above figures. From **Fig. 2**, we can find that the maximum errors of all simplified depletion chain calculations are bounded between -200pcm and 200pcm.

Target nuclides' number densities of different depletion chain calculations are shown in **Fig. 3** to **Fig. 5**.

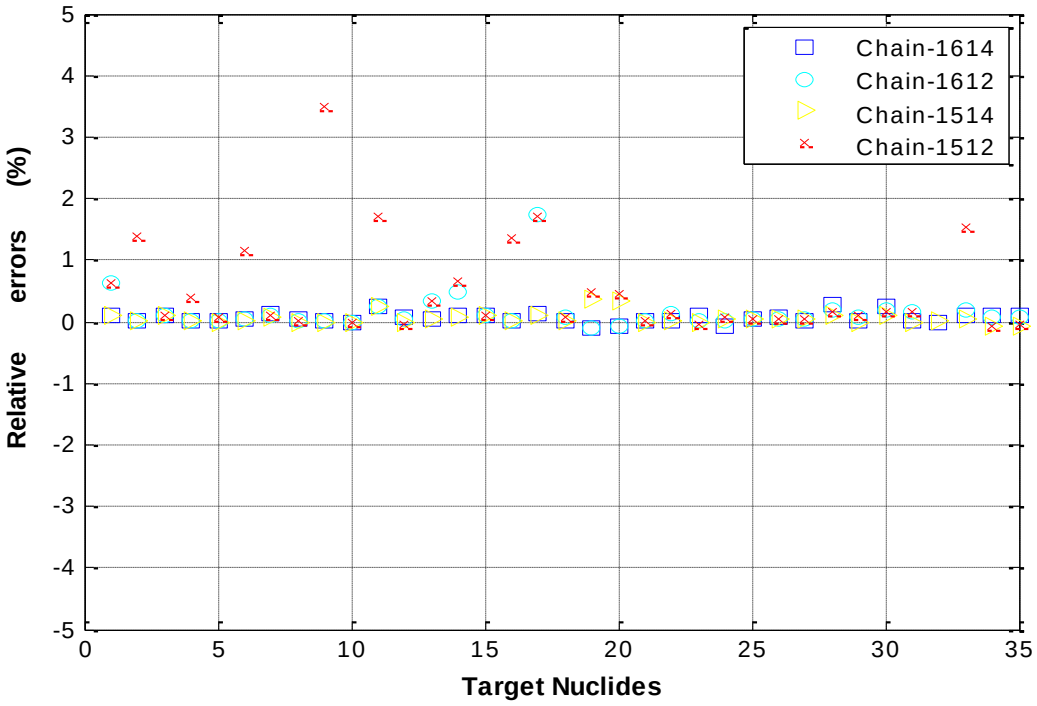

Fig 3. Relative errors of target nuclides number densities at Burnup 1GWd/tHM

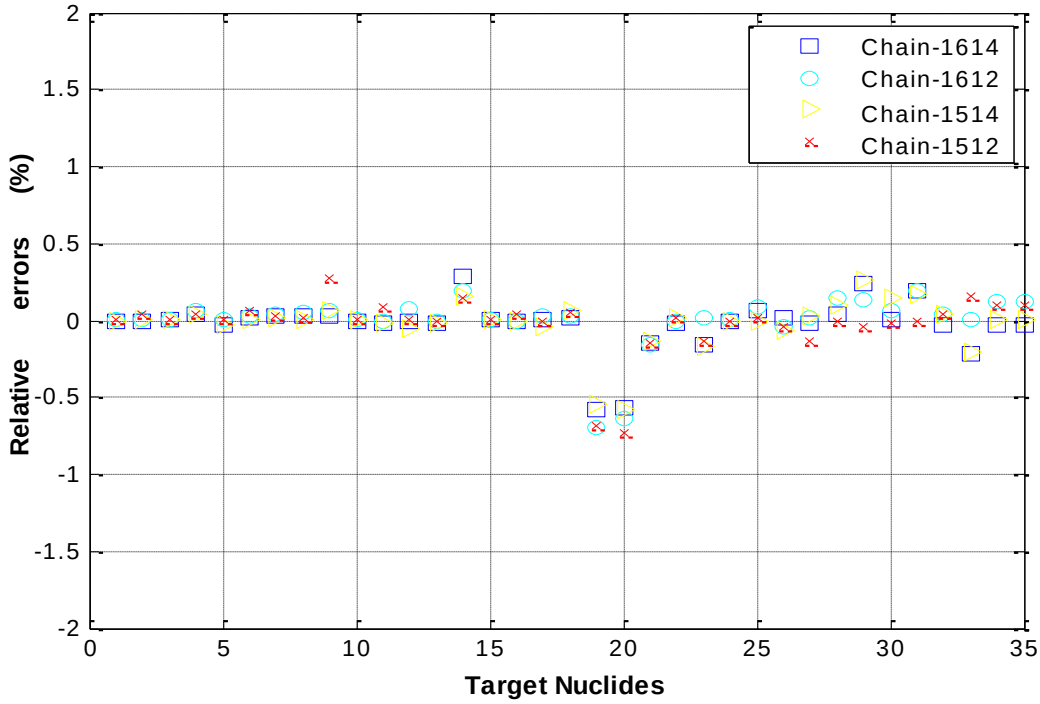

Fig 4. Relative errors of target nuclides number densities at Burnup 40GWd/tHM

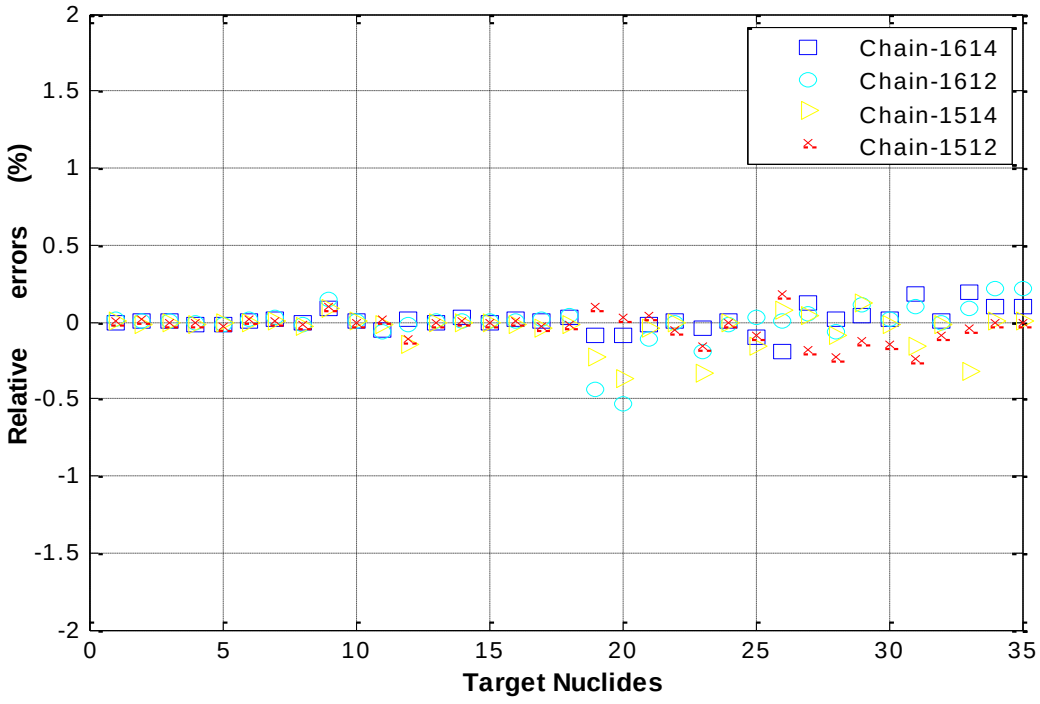

Fig 5. Relative errors of target nuclides number densities at Burnup 70GWd/tHM

Although, there are also stochastic errors in the nuclide number density results, satisfactory accuracy is achieved. For the most simplified depletion chain, which is Chain-1512, the absolute relative errors of all target nuclides are below 4% at 1 GWd/tHM, the maximum absolute relative errors drop to less than 1% at 40 GWd/tHM and 70 GWd/tHM. The higher error level at first few steps is due to vast changes of spectrum during irradiation startup period.

Time and storage consumptions are shown in the table below. And 48 cores are used for the MPI-parallel neutronic calculation.

Table 3. Calculation depletion chains

Chain name	Storage per core (MB)	Time spent in one neutronic calculation (average, s)
Reference	329	639.77
Chain-1614	226	327.19
Chain-1612	226	321.17
Chain-1514	155	254.50
Chain-1512	152	248.04

Since only one depletion region is involved, the time and storage requests of depletion calculation are negligible. The savings for simplified depletion chain calculations are mainly due to the reduction of the number of traced nuclides in neutronic calculation.

5. CONCLUSIONS

In this paper, a new depletion chain simplification method is proposed and tested. The method relies on detailed significance analysis of reaction channels and decay nuclides. Numerical results suggest that the method can effectively reduce the time and storage consumptions in depletion calculation, while preserving intended accuracy requirements. The method will be tested on multi depletion region problems, such as assembly calculation. Also, the parameters utilized are conservative, and optimization work should be carried out to further strength the effectiveness of the method.

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