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Improvements to the Transmutation Trajectory Analysis of depletion evaluation

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ABSTRACT

To simulate the nuclide evolution process in a nuclear reactor core, the Transmutation Trajectory Analysis (TTA) method solves the depletion equations by decomposing the depletion system into a number of linear chains and then solving each one analytically. In this paper, two improvements are proposed for TTA to obtain better efficiency. Firstly, the pseudo node evaluation for linear chain cutoff check has been removed. Instead, a time-averaged nuclide number density is employed as the chain termination criteria, which in theory can improve the computational efficiency by a factor of two. Secondly, a new recursive formula has been derived to replace the legacy direct solution formula for solving the linear chains. Numerical tests have been carried out based on a typical PWR fuel cycle to demonstrate that these improvements enable the TTA method to solve decay problems efficiently and accurately.

1. Introduction

Nuclear energy release is accompanied by nuclides depletion process. The variety of nuclides vary in their toxicities, decay properties and microscopic cross sections. Therefore, predicting the time evolution of nuclide inventories is of vital importance in nuclear applications. Actually, the depletion process is coupled together with both neutronics and thermal–hydraulics processes. Within a small enough time step, however, these three processes can be treated independently. Although the depletion process is quite complicated, there are governing equations called depletion equations describing the variation rate of nuclide number density which equal the difference of rate of production and consumption. These equations can be written as a set of first order ordinary differential equations assuming constant microscopic reaction rates (Stamm'ler and Abbate, 1983) for each depletion region during small time steps. The coefficient matrix of the depletion equations, or depletion matrix, describes the nuclide transformation relations. For example, each of the diagonal entries stands for the disappearance of the corresponding nuclide, while each of the off-diagonal entries represents the contribution between two different nuclides.

There are two major types of methods which can be used for solving the depletion equations with constant coefficients: matrix exponential methods and linear chain methods. In general, computation of matrix exponential in itself constitutes a rich field of study (Moler and Van Loan, 2003). Several methods have been introduced to solving depletion equations, such as the Taylor expansion and truncation method with secular equilibrium assumed for short-lived nuclides (Croff, 1980; Hermann and Westfall, 1998), and Chebyshev rational approximation method (CRAM) (Pusa and Leppänen, 2010; Pusa, 2011). Taylor expansion and truncation method is based on the definition of the matrix exponential in Taylor series form. CRAM is related to the rational approximation of exponential function (Trefethen et al., 2006). Other than these matrix approaches, linear chain methods offer a direct solution method. With little computational overhead, this approach explicitly models nuclide chains and enumerates all important ones. A more recent general analytical solution by Cetnar, referred to as Transmutation Trajectory Analysis method (TTA) (Cetnar, 2006) has remedied the identical vanishing coefficients issue. When this solution is used, the only approximation left is the termination of linear chains of low importance. The term linear chain here refers to a simple depletion process in which each nuclide has at most only one predecessor and at most only one daughter nuclide. Each of these linear chains is governed by analytically solvable bi-diagonal depletion equations, or bi-diagonal Bateman equations. The solution of the original depletion equations can be obtained as a superposition of those analytical solutions.

The depletion problems could be classified into two different types, namely the decay problems and the burnup problems (Isotalo, 2013), based on the absence or presence of neutron flux.

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For a pure decay system, the disassembly of the directed graph representing the depletion matrix called linearization would be exact since a finite number of linear chains with finite length will be equal to the original depletion equations according to the superposition principal and the absence of closed transformation cycles. The latter condition is insured, since a nuclide could not go through a series of energy emitting decay processes and return to itself precisely with an unchanged mass. However, for a burnup system with neutron-induced nuclear reactions involved, there might be closed transformation cycles, thus a finite or even infinite number of linear chains with infinite length are necessary for maintaining the equivalence between the original depletion equations and the series of linear chains. Practically, not all of these linear chains are important enough to be considered however, because the number of nuclides transferred through the linear chain decreases rapidly along the chain. Consequently, a cutoff check is carried out to determine the effective end of each linear chain growing process. Considering that the determination of linear chain solutions contributes most to the computational cost, the efficiency could be improved by reducing the number and the length of calculated linear chains or finding more efficient analytic formulas to resolve the nuclide number densities for each of these linear chains. Such an efficiency improvement would accumulate considerable saving on computational effort in applications that demand large numbers of depletion calculations.

In this paper, two improvements concerning efficiency of TTA are proposed. Firstly, a time-averaged nuclide number density is employed to simplify the linear chain cutoff check, which is usually done by calculating the number density of a stable node appended at the end of the chain. In this paper, this artificial stable node is referred to as a pseudo node. Secondly, in terms of the analytic solution, a recursive formula, which is mathematically equivalent with the legacy direct formula, is derived and implemented to reduce computational effort spent on solving linear chains. Numerical tests have been carried out based on a typical PWR fuel cycle. It has been demonstrated that these improvements could make the TTA method run faster by a factor of about 8 while maintaining the same computational accuracy. While it has been shown that the burnup problems could be solved elegantly by CRAM (Pusa and Leppänen, 2010; Pusa, 2011; Isotalo and Aarnio, 2011), the TTA method has better performance for solving decay problems, and could be viewed as a complement with respect to CRAM.

The paper is organized as the following. Section 2 derives the theory and formulas of the two improvements in detail. Numerical results and discussions of three selected test cases based on a PWR fuel cycle are given in Section 3. Finally, conclusions are drawn in Section 4.

2. Theoretical model

The TTA method finds the final solution by summing up contributions from all linear chains. The basic building element of linear chain is called node, and each root node corresponds to a nuclide with non-zero initial number density. The level of a node is defined as its distance from the root node. These concepts are illustrated in Fig. 1, in which only nuclide a is assigned a non-zero initial number density for the sake of simplicity. The linear chain searching process is in a form of three levels of iterations. The outermost iteration selects the nuclides that have non-zero initial nuclide number densities as root nodes. The second level iteration is composed of two innermost iterations: one for growing the linear chain along the transfer relationships until being terminated; and the other for identifying the restart node, which is defined as the node that has unexplored successors and is closest to the last node. Between the two innermost iterations, the nodes after restart node of the linear chain are taken into account to the contributions of the solution, since they belong to the newly explored transmutation path. Termination of linear chain in the growing process happens when the last node has no successors or the importance of the linear chain falls below a certain value (cutoff criterion). The second level iteration ends when the restart node cannot be found. The pseudo code of the linear chain searching process is provided in Appendix A under Algorithm 1.

The governing equations for each linear chain are the bi-diagonal Bateman equations:

$$\frac{dN_1(t)}{dt} = -\lambda_1 N_1(t) \tag{1a}$$

$$\frac{dN_{i+1}(t)}{dt} = \lambda_{i+1,i} N_i(t) - \lambda_{i+1} N_{i+1}(t) \quad (1 \leqslant i < n) \tag{1b}$$

where $N_i(t)$ refers to the number density (cm^{-3}) of the ith node, λ_i is the vanishing coefficient of ith node nuclide (s^{-1}), while $\lambda_{i+1,i}$ stands for the transfer coefficient from the ith node nuclide to $(i+1)$th node nuclide, defined as:

$$\begin{aligned} \lambda_i &= \lambda_i^{\text{decay}} + \sigma_{a,i}\phi \\ \lambda_{i+1,i} &= b_{i+1,i}\lambda_i^{\text{decay}} + \sigma_{i+1,i}\phi \end{aligned} \tag{2}$$

λ_i^{decay} is the decay constant, $\sigma_{a,i}$ is the single group microscopic absorption cross section, $b_{i+1,i}$ and $\sigma_{i+1,i}$ are the branching ratio and the single group microscopic cross section that produces $(i+1)$th node nuclide respectively, ϕ is the neutron flux.

2.1. Improvement on the cutoff check

To avoid linear chains of infinite length, or unnecessary linear chain nodes, a criterion has to be employed to stop the searching process for each linear chain. The essential measurement is the linear chain passage (Cetnar, 2006; Isotalo and Aarnio, 2011), which is defined as the number density that goes through the last transfer relation:

$$P_n = \int_0^{t_f} \lambda_{n+1,n} \cdot N_n(t) dt \tag{3}$$

where the linear chain is cut between the nth and the $(n+1)$th nodes, and $\lambda_{n+1,n}$ is the corresponding transfer coefficient. It offers an estimate of the remaining number densities that will be neglected. Thus, the linear chain should be terminated once P_n falls below the cutoff criterion determined by:

$$\varepsilon_{\text{cutoff}} = \text{cutoff} \cdot N_{\text{total}}(0) \tag{4}$$

where $N_{\text{total}}(0)$ represents the initial total nuclide number density.

The independent pseudo node approach, which is implemented initially, appends a pseudo node with $\lambda_{\text{pseudo}} = 0.0$ and $\lambda_{\text{pseudo},n} = 1.0$ after the nth node of the linear chain. Then, it can be shown that P_n equals $\lambda_{n+1,n} N_{\text{pseudo}}(t_f)$. Since most nodes are not stable, and require pseudo node calculations, the total computing effort is nearly doubled.

An alternative approach is to determine linear chain passage from a time-averaged nuclide number density:

$$\overline{N}_n(t) = \frac{1}{t}\int_0^t N_n(\tau) d\tau \tag{5}$$

As will be discussed latter, $N_n(t)$ could be expanded as the sum of terms taking the form $t^k e^{-\lambda_j t}$. The integrals of these terms could be pre-calculated and stored for all possible combinations of λ_j and k up to a very limited number of values (3 is enough in most cases). Compared to the independent pseudo node approach, the computation solving the pseudo node is saved, and additional integration is required. The time saving effect dominates in practice, because the integration is merely based on weighted summation of pre-calculated values, therefore the computational time is approximately