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Algorithms of solving the burnup equation with external feed

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ABSTRACT

Burnup calculation is an essential task in nuclear reactor physics. Burnup equation is generally used to describe the generation, depletion and decay process in the nuclide system. In some nuclide systems, there may exist physical or chemical exchange with the surroundings, such as the spent fuel reprocessing facilities and some advanced reactors with continuous refueling and discharging like the liquid-metal-fuel reactor. This work studies the burnup calculations with considering external feed. Two external feed models, that is the relative feed and the absolute feed, are addressed. The burnup equations with external feed are solved by utilizing the variation of transmutation trajectory analysis (TTA) method and matrix exponential methods. The proposed models and methods have been implemented in the NUIT (NUclide Inventory Tool) code. Various test cases are calculated for validation, and the numerical results are satisfactory.

1. Introduction

Burnup calculation is an important aspect of nuclear reactor physics, which evaluates the changes of the isotopic compositions and the relevant physical quantities, e.g. the reaction rates, radioactivity, decay heat and etc. The burnup equation describes the change rates of the nuclide density, which is usually in the form of first-order differential equation with constant coefficients. The algorithm of solving the burnup equation mainly includes two categories, that is the transmutation trajectory analysis (TTA) method (Bateman, 1910) and the matrix exponential methods (Pusa, 2011). TTA is able to provide analytical solution in the decay system, however, its accuracy and efficiency deteriorates in the burnup systems with cyclic chains. One matrix exponential method is the Taylor series expansion method that was implemented in the ORIGEN code (Croff, 1980). The Taylor series method has drawbacks in dealing with the short-lived nuclides, due to a large norm of the transition matrix. In recent years, some advanced matrix exponential methods have been proposed to solve the burnup equation with correctly treating short-lived nuclides. Those methods include the Chebyshev rational approximation method (CRAM) (Pusa, 2011), the Quadrature-based rational approximation method (QRAM) (Trefethen et al., 2006), the Laguerre polynomial approximation method (LPAM) (She et al., 2012), and the Mini-max polynomial approximation method (MMPA) (Yosuke et al., 2015).

In some nuclide system, such as the spent fuel reprocessing facilities and some advanced reactors with continuous refueling and discharging (e.g. the liquid-metal-fuel reactor), we need to consider the physical or chemical external feed (or removal) in burnup calculations. As a result, special algorithms should be investigated to solve such kind of burnup equations. The burnup equation with continuous feed in a constant rate has been considered in the depletion code KORIGEN (Fischer et al., 1991) and ORIGEN-S (Gauld, 2011), which is solved by the truncated Taylor seizes method. Recently, CRAM has been utilized for the burnup equation with external feed (Isotalo and Wieselquist, 2015), which is based on converting the original transition matrix to an augmented matrix.

NUIT (NUclide Inventory Tool) is a newly-developed radioactive nuclide inventory code for HTGR by Institute of Nuclear and New Energy Technology (INET) (Li et al., 2017). NUIT has employed most of existing burnup solvers including TTA, CRAM, QRAM, LPAM and MMPA, and it is capable to deal with decay calculation, constant flux calculation and constant power calculation. Base on the NUIT code, study on the algorithms of solving burnup equation with external feed has been performed in this paper. Two external-feed models are proposed, which are mathematically expressed in homogeneous and nonhomogeneous forms of burnup equations, respectively. Then, the burnup equations with accounting for external feed are solved by utilizing the variation of TTA and CRAM methods. The validity and accuracy of the proposed methods has

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been examined by various numerical examples, which give satisfactory results.

The remainder of the paper is organized as follows. Section 2 describes the mathematical models of the burnup equations with accounting for the external feed. Section 3 introduces the algorithms of treating different kinds of the external feed. Numerical results of various test cases are presented in Section 4. Concluding remarks are given in Section 5.

2. Mathematical model

2.1. Conventional burnup equation

The conventional burnup equations consist of a set of first-order liner differential equations, which can be written as

$$\frac{dn_i}{dt} = \sum_{i \neq j} b_{j,i}^{eff} \lambda_j^{eff} n_j - \lambda_i^{eff} n_i \tag{1}$$

where n_i is the concentration of nuclide i; λ_i^{eff} is the effective decay constant of nuclide i, $b_{i,j}^{eff}$ is the effective branching ratio for the transmutation of nuclide i to nuclide j. Coefficients λ_i^{eff} and $b_{i,j}^{eff}$ can be obtained with the following equation:

$$\begin{cases} \lambda_i^{eff} = \lambda_i + \phi \sum_j \sigma_{i,j} \\ b_{i,j}^{eff} = (b_{i,j}\lambda_i + \sigma_{i,j}\phi)/\lambda_i^{eff} \end{cases} \tag{2}$$

where λ_i is the decay constant of nuclide i, ϕ is the neutron flux, and $\sigma_{i,j}$ is the microscopic one-group cross-section.

Burnup equations in Eq. (1) can be written in a matrix form:

$$\begin{cases} \frac{d\mathbf{n}}{dt} = \mathbf{An} \\ \mathbf{n}(0) = \mathbf{n}_0 \end{cases} \tag{3}$$

where $\mathbf{n}(t) \in R^n$ is the isotopic concentration vector of the considered burnup chains and $\mathbf{A}$ is the transition matrix containing the decay and transmutation coefficients of the nuclides under consideration.

2.2. Burnup equation with external feed

In this paper, two kinds of external-feed models are considered, which are referred as the relative feed and absolute feed, respectively.

The relative feed means that the external feed is proportional to the nuclide concentration. For example, in some liquid-metal-fuel reactors, fission products are continuously removed from the reactor core in order to improve the neutron economy, and the removal rate is usually described as the percentage of the nuclide's present concentration. In mathematics, it leads to changing the effective decay constant λ_i^{eff} in the burnup equation:

$$\begin{aligned} \frac{dn_i}{dt} &= \sum_{i \neq j} b_{j,i}^{eff} \lambda_j^{eff} n_j - \lambda_i^{eff} n_i + r_i n_i \\ &= \sum_{i \neq j} b_{j,i}^{eff} \lambda_j^{eff} n_j - (\lambda_i^{eff} - r_i) n_i \end{aligned} \tag{4}$$

where r_i is the relative feed rate of nucliden_i.

Correspondingly, the matrix format of Eq. (4) can be written as

$$\begin{cases} \frac{d\mathbf{n}}{dt} = [\mathbf{A} + diag(r_i)]\mathbf{n} = \mathbf{An} \\ \mathbf{n}(0) = \mathbf{n}_0 \end{cases} \tag{5}$$

where $\mathbf{A}$ is a variant of transition matrix, whose diagonal elements have been adjusted according to the relative feed rate.

Different from the relative feed, the absolute feed model represents that the external feed rate is a fixed value. For example, in the equilibrium state of pebble-bed HTGR, fresh fuel is continuously fed into the core with a fixed rate. The absolute feed model introduces a nonhomogeneous term into the burnup equation, leading to the following form:

$$\frac{dn_i}{dt} = \sum_{i \neq j} b_{j,i}^{eff} \lambda_j^{eff} n_j - \lambda_i^{eff} n_i + s_i \tag{6}$$

where s_i is the absolute feed rate of nuclide i.

The matrix form of nonhomogeneous term is as follows:

$$\begin{cases} \frac{d\mathbf{n}}{dt} = \mathbf{An} + \mathbf{s} \\ \mathbf{n}(0) = \mathbf{n}_0 \end{cases} \tag{7}$$

where $\mathbf{s}$ is the vector of absolute feed rate in term of nuclide.

Noting that the signs of external feed terms have no limitation in mathematics, the above models are essentially able to account for positive or negative feed rate for any nuclide. If the feed rate is negative, it means an external removal rate in physics. However, an improper removal rate in Eq. (6) may cause the burnup equation has negative solution in mathematics, which does not have physical meanings.

3. Burnup algorithms

3.1. Conventional burnup algorithms

3.1.1. Transmutation trajectory analysis (TTA)

TTA method (Isotalo and Aarnio, 2011) solves the burnup equation by first decomposing the complicated burnup chains into a set of linear chains, and then solving each linear chain independently. Assuming that only the first nuclide (or the head nuclide) of the linear chain has a non-zero initial nuclide density $n_1(0)$, thus, the concentration of the n-th nuclide along the linear chain can be analytically expressed as

$$n_k(t) = n_1(0) B_k \sum_{i=1}^{k} \alpha_i^k e^{-\lambda_i^{eff} t} \tag{8}$$

Eq. (8) is the general solution of the burnup Eq. (1) utilizing TTA method, where B_k and α_i^k are the coefficients written as

$$B_k = \prod_{j=1}^{k-1} b_{j,j+1}^{eff} \tag{9}$$

$$\alpha_i^k = \frac{\prod_{j=1}^{k-1} \lambda_j^{eff}}{\prod_{j=1, j \neq i}^{k} (\lambda_j^{eff} - \lambda_i^{eff})} \tag{10}$$

TTA method is essentially an analytical method, which has been successfully applied in decay calculations with high precision and efficiency. Nevertheless, the computation time of TTA method can easily become excessive if all chains are followed until a stable nuclide is encountered, and cutoffs have to be introduced to terminate insignificant chains (Huang et al., 2016).

3.1.2. Matrix exponential methods

Solutions of the matrix-form burnup equations (Eq. (3)) can be expressed by the matrix exponential:

$$\mathbf{n}(t) = e^{\mathbf{A}t} \mathbf{n}_0 \tag{11}$$

where $e^{\mathbf{A}t}$ is the matrix exponential. The essence of all kinds of matrix exponential methods is to compute the matrix exponential $e^{\mathbf{A}t}$, by means of rational approximation or polynomial expansion.