Comparison of Two-Block Decomposition Method and Chebyshev Rational Approximation Method for Depletion Calculation

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1. Introduction

The accurate prediction of the time-dependent nuclide concentrations in a nuclear fuel is important to evaluate many issues, e.g., the neutron multiplication factor in criticality safety, neutron and gamma-ray sources in radiation shielding, and radiotoxicity and heat load evaluation in spent fuel repository, etc. [1]. In practice, those source-term analyses are performed via the depletion codes, e.g., ORIGEN. Such a code uses approximate techniques (e.g., secular equilibrium) for short-lived nuclides in order to perform the calculations efficiently [2]. The code gives inaccurate results of nuclides for evaluation of source term analysis, e.g., Sr-90, Ba-137m, Cs-137, etc.

A Krylov Subspace method was suggested by Yamamoto et al. [3]. The method is based on the projection of solution space of Bateman equation to a lower dimension of Krylov subspace. It showed good accuracy in the detailed burnup chain calculation if dimension of the Krylov subspace is high enough. However, it requires considerable computing time when the short-lived nuclides are involved in the burnup chain.

Recently, Chebyshev rational approximation method (CRAM) [4] and two-block decomposition (TBD) method [5] were proposed for accurate and efficient depletion calculations of very detailed burnup chains. Since the two methods showed good accuracy in the detailed burnup chain given in each work [4, 5], the methods would show results with similar accuracy for the given test problem. In this paper, we will compare the two methods in terms of accuracy and computing time.

2. Chebyshev Rational Approximation and Two-Block Decomposition Methods for Depletion Calculation

2.1 Chebyshev Rational Approximation Method

According to Ref. 6, rational function is known to be a good approximation to the function, e^{-x} in $[0, \infty)$. Rational approximation in the partial fraction decomposition form is expressed as :

$$r_{k,k}(x) = \alpha_0 + \sum_{j=1}^{k} \frac{\alpha_j}{x-\theta_j}, \tag{1}$$

where
α_0 *:* limit of the function $r_{k,k}$ at infinity,
α_j *:* residues at the poles θ_j (form conjugate pairs).

Computing cost for Eq. (1) can be reduced to half for a real variable as

$$r_{k,k}(x) = \alpha_0 + 2\,\mathrm{Re}\left(\sum_{j=1}^{k/2} \frac{\alpha_j}{x-\theta_j} \right). \tag{2}$$

In the matrix form for depletion calculation [4], Eq. (2) is expressed as :

$$\begin{aligned} \vec{X} &= r_{k,k}(At)\,\vec{X}(0) \\ &= \alpha_0 \vec{X}(0) + 2\,\mathrm{Re}\left(\sum_{j=1}^{k/2} \alpha_j \left(At - \theta_j I\right)^{-1} \vec{X}(0) \right). \end{aligned} \tag{3}$$

Coefficients, α_j's, are determined by using a Remez-type algorithm applying to the following equation [6] :

$$\sup_{x\in R} \left| \hat{r}_{k,k}(x) - e^{-x} \right| = \inf_{r_{k,k}\in\pi_{k,k}} \left\{ \sup_{x\in R} \left| r_{k,k}(x) - e^{-x} \right| \right\}. \tag{4}$$

Using a predetermined set of the coefficients, matrix exponential can be performed. The algorithm is implemented in EXPOKIT [7].

2.2 Two-Block Decomposition Method

Depending on the magnitude of the "effective" decay constant of nuclide *i* :

$$\lambda_i^{eff} = \lambda_i + \sum_{r=f,c} \sigma_r \phi, \tag{5}$$

the system of Bateman equations are decomposed into short-lived and long-lived blocks as :

$$\dot{\vec{X}}_S = A_S \vec{X}_S + A_{SL} \vec{X}_L, \tag{6a}$$

$$\dot{\vec{X}}_L = A_L \vec{X}_L + A_{LS} \vec{X}_S, \tag{6b}$$

The two blocks are calculated separately, but with coupling. Due to very large norm of A_S, Eq. (6a) is solved by the general solution of Bateman equation [8] for each nuclide in the short-lived block.

In order to reduce computation burden in Bateman solution calculations, an "importance" concept is introduced for selecting important nuclides that produce a particular short-lived nuclide. [5].

Consider the reaction chain involving production of short-lived nuclide *s* shown in Fig. 1.

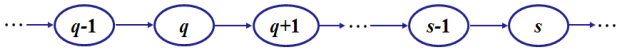

Fig. 1. Example of Reaction Chain

The importance of parent *q* for production of short-lived nuclide *s* from time *t* to $t+\Delta t$, $\mathrm{IMP}_{s,q}(t,t+\Delta t)$, is defined as :

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$$\mathrm{IMP}_{s,q}(t,t+\Delta t) \equiv \frac{\frac{a_{s,s-1}}{\lambda_{s-1}^{eff}} \int_{t}^{t+\Delta t} \lambda_{s-1}^{eff} x_{s-1,q}(\tau) d\tau}{\int_{t}^{t+\Delta t} \lambda_{s}^{eff} \sum_{i=q+1}^{s} x_{s,i}(\tau) d\tau + \sum_{i=q+1}^{s} x_{s,i}(t+\Delta t)}, \quad (7)$$

where

$$x_{s,q}(\tau) = \frac{1}{\lambda_s^{eff}} \prod_{\substack{j=1 \\ j\neq s}}^{n} \left(\frac{a_{i,j}}{\lambda_j^{eff}} \right) \sum_{i=1}^{n} \lambda_i^{eff} \prod_{\substack{j=1 \\ j\neq i}}^{n} \left(\frac{\lambda_j^{eff}}{\lambda_j^{eff} - \lambda_i^{eff}} \right)^{m_j} \cdot \exp\left(-\lambda_i^{eff} (\tau - t) \right) \Lambda_{i,\mu_i}, \quad (8)$$

$$\Lambda_{i,\mu_i} = \sum_{m=0}^{\mu_i} \frac{\left(\lambda_i^{eff} (\tau - t) \right)}{\lambda_s^{eff}} \cdot \sum_{l=0}^{\mu_i} \sum_{h_1=0}^{\mu_i} \cdots \sum_{h_n=0}^{\mu_i} \prod_{\substack{j=1 \\ j\neq s}}^{n} \binom{h_k + \mu_k}{\mu_k} \cdot \left(\frac{\lambda_i^{eff}}{\lambda_i^{eff} - \lambda_k^{eff}} \right) \delta\left(\mu_i - m, l + \sum_{\substack{k=1 \\ k\neq i}}^{n} h_k \right). \quad (9)$$

The nuclide q is selected as an important nuclide for production of short-lived nuclide s if $\mathrm{IMP}_{s,q}(t,t+\Delta t)$ is larger than a criterion (IMP) set by the user.

With only important parents for the short-lived nuclide s, general Bateman solution is written as:

$$x_s(\tau) = \sum_{j=1}^{n_{IMP}} \frac{x_{j0}}{\lambda_s^{eff}} \prod_{\substack{j=1 \\ j\neq s}}^{n_{IMP}} \left(\frac{a_{i,j}}{\lambda_j^{eff}} \right) \sum_{i=1}^{n_{IMP}} \lambda_i^{eff} \prod_{\substack{j=1 \\ j\neq i}}^{n_{IMP}} \left(\frac{\lambda_j^{eff}}{\lambda_j^{eff} - \lambda_i^{eff}} \right)^{m_j} \cdot \exp\left(-\lambda_i^{eff} (\tau - t) \right) \Lambda_{i,\mu_i}, \quad (10)$$

where

$x_s(\tau) \in \vec{X}_S(\tau)$,

n_{IMP}: number of important nuclides determined by importance calculation, ($n_{IMP} \le n$).

Meanwhile, the solution of long-lived block, Eq. (6b) is expressed as :

$$\vec{X}_L(t+\Delta t) = \exp\left[A_L \Delta t\right] \vec{X}_L(t) + \exp\left[A_L \Delta t\right] \left[\sum_{i=1}^{G_n} w_i \exp(-A_L \tau_i) A_{LS} \vec{X}_S(\tau_i) \right], \quad (11)$$

where

G_n: number of Gaussian quadrature set,

w_i: weights for Gaussian quadrature, $\sum_{i=1}^{G_n} w_i = \Delta t$,

τ_i: abscissas for Gaussian quadrature, $\tau_i \in [t, t+\Delta t]$.

In contrast to A_S in Eq. (6a), the norm of A_L is small enough to calculate matrix exponentials efficiently in Eq. (11).

3. Numerical Results

In order to get a realistic initial condition, 3.19w/o enriched PWR fuel is burned for 100 days by the ORIGEN code [1] with Δt=20 days. Then, CRAM and TBD are compared for a depletion calculation of the fuel irradiated by constant neutron flux 1.98E+14#/cm^2-sec for 20 days. The burnup matrix consists of 976 nuclides. Reference calculation is per-formed by simple Taylor series expansion with the ORIGEN code using a small time step (Δt=2.0E-07 days) and a large number of expansion terms (70 terms). Computing time of the reference calculation is 1.668E+05 sec (~1.30 days) on Intel i5 2.67-GHz CPU.

The magnitude of the effective decay constant used for decomposition is $\lambda_i^{eff} \times \Delta t = |\ln(0.001)| \sim 6.9$ (as used in ORIGEN 2.2 for its own treatment of short-lived nuclides). With the time step of Δt =20 days, there are 670 short-lived nuclides in the TBD. The TBD calculations are performed for various IMPs with a fixed number of G_n (G_n=20).

Meanwhile, CRAM calculation is also performed with Δt =20 days. In the CRAM, there is no decomposition of short- and long-lived blocks, i.e., concentration of all nuclides are calculated via Eq. (3).

The maximum and relative RMS errors obtained by the two methods are listed in Table 1. Computation times of the two methods are also listed in Table 2.

Table 1. Maximum and relative RMS errors from TBD and CRAM

	Importance (IMP)	Maximum error (%)	Relative RMS
TBD	1.0E+00	1.593E+00	9.553E-02
	1.0E-01	1.189E-01	8.757E-03
	1.0E-02	1.692E-02	1.504E-03
	1.0E-03	3.219E-03	2.894E-04
	1.0E-04	3.219E-03	2.890E-04
	1.0E-05	3.219E-03	2.894E-04
	1.0E-06	3.219E-03	2.894E-04
	1.0E-07	3.219E-03	2.894E-04
	1.0E-10	3.219E-03	2.894E-04
	1.0E-20	3.219E-03	2.894E-04
CRAM	N/A	5.470E-03	3.031E-04

Table 2. Computation times of the TBD and CRAM

	Importance (IMP)	Computing time (sec)
TBD	1.0E+00	0.21
	1.0E-01	0.31
	1.0E-02	0.43
	1.0E-03	0.51
	1.0E-04	0.71
	1.0E-05	0.83
	1.0E-06	1.03
	1.0E-07	1.51
	1.0E-10	1.72
	1.0E-20	3.35
CRAM	N/A	0.23

Sufficient accuracies in relative RMS errors and maximum errors are obtained by the TBD (3.219E-03 in the maximum error, 2.890E-04 in RMS error) with sufficient IMP (IMP≤1.0E-03). Computation time of the method for IMP=1.0E-03 and Δt=20 days is 0.51 sec. With the sufficient IMP (IMP≤1.0E-03), the TBD shows better accuracy (3.219E-03 in the maximum error, 2.890E-04 in RMS error) than that of the CRAM (5.4670E-03 in the maximum error, 3.031E-04 in RMS error). However, computation time of the TBD (0.51 sec) is slightly longer than that of the CRAM (0.23 sec).

The TBD results (IMP=1.0E-03), and the CRAM results are compared for the similar accuracy. The relative errors of 9 important nuclides for source-term analysis are shown in Table 3.

In the CRAM results, the 9 nuclides show the maximum errors of 9.271E-03%, while the TBD shows the reduced maximum errors of 4.262E-03%.

Table 3. Relative errors from TBD and CRAM and importance of the listed nuclides

Nuclides	Relative error (%)		Importance
	TBD	CRAM	
Se-79	8.986E-07	9.272E-07	Important dose contributor in high level waste repository
Kr-85	1.112E-06	1.034E-06	Decay heat source
Sr-90	-1.072E-05	-1.072E-05	One of the top decay heat source
Rh-106	2.26E-05	3.243E-05	Strong γ-ray source
Cd-113m	3.274E-06	2.263E-06	The most concern at DOE's reprocessing sites such as Hanford
Ba-140	4.262E-03	5.243E-03	High activity after several months of post-irradiation cooling
La-140	1.318E-02	9.271E-03	
Sm-152	2.769E-03	3.451E-03	Criticality safety evaluation for spent fuel
Eu-153	3.228E-06	2.114E-06	

4. Conclusions

In this paper, two-block decomposition (TBD) method and Chebyshev rational approximation method (CRAM) are compared in the depletion calculations. In the two-block decomposition method, according to the magnitude of effective decay constant, the system of Bateman equation is decomposed into short- and long-lived blocks. The short-lived block is calculated by the general Bateman solution and the importance concept. Matrix exponential with smaller norm is used in the long-lived block. In the Chebyshev rational approximation, there is no decomposition of the Bateman equation system, and the accuracy of the calculation is determined by the order of expansion in the partial fraction decomposition of the rational form. The coefficients in the partial fraction decomposition are determined by a Remez-type algorithm.

The two methods are comparable in performance. With sufficient values of importance, the two-block decomposition method shows better accuracy than the Chebyshev rational approximation method. However, the Chebyshev rational approximation method shows slightly faster computation time than the two-block decomposition method.

Considering that the two-block decomposition method can be further optimized, computation times of the method could be reduced further than those shown in this study, maintaining its superiority in accuracy.

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