Journal of the Korean Nuclear Society
Volume 31, Number 2, pp.172~181, April 1999

Comparison of Matrix Exponential Methods for Fuel Burnup Calculations

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(Received July 4, 1998)

Abstract

Series expansion methods to compute the exponential of a matrix have been compared by applying them to fuel depletion calculations. Specifically, Taylor, Padé, Chebyshev, and rational Chebyshev approximations have been investigated by approximating the exponentials of burn matrices by truncated series of each method with the scaling and squaring algorithm. The accuracy and efficiency of these methods have been tested by performing various numerical tests using one thermal reactor and two fast reactor depletion problems. The results indicate that all the four series methods are accurate enough to be used for fuel depletion calculations although the rational Chebyshev approximation is relatively less accurate. They also show that the rational approximations are more efficient than the polynomial approximations. Considering the computational accuracy and efficiency, the Padé approximation appears to be better than the other methods. Its accuracy is better than the rational Chebyshev approximation, while being comparable to the polynomial approximations. On the other hand, its efficiency is better than the polynomial approximations and is similar to the rational Chebyshev approximation. In particular, for fast reactor depletion calculations, it is faster than the polynomial approximations by a factor of ~1.7.

1. Introduction

In fast reactor core designs, high burnup is an important objective to reduce the fuel cycle cost. In order to assure fuel pin integrity in a high burnup core without introducing additional design margins, it is necessary to predict the burnup history of each fuel pin accurately. Furthermore, in the fast reactor fuel cycle accompanying the reprocessing of spent fuel, the burnup and isotope distribution of spent fuel has a large effect on the composition of the refabricated fuel, and it is also important for the accountancy and control of fuel material required in the reprocessing process. In this case, spatially detailed nuclide densities (e.g. by axial position for individual fuel pins) are required when pre-calculated fits of number densities for a limited number of "enveloping" depletion histories are unavailable or inadequate. The required computational effort is particularly large when the pin-wise density distributions are needed for a large number of nuclides. This has motivated the investigation of more efficient and accurate computational methods for performing fuel depletion.

Generally, all depletion methods rely upon the quasi-static approximation in which the nonlinear neutron and nuclide fields are decoupled for a subinterval of the burn cycle.[1] The nuclide transmutation equation is then solved by approximating the time-dependent flux over each subinterval using a constant value (e.g., a weighted average of the beginning and the end of subinterval fluxes). In this case, the nuclide transmutation equation is represented by a system of first-order differential equations. The formal solution of this depletion equation is obtained in terms of the exponential of the transmutation matrix. This exponential function of the transmutation matrix is typically determined by a Taylor series approximation. This technique is currently used in the codes ORIGEN[2], REBUS-3[3], and BURNER[4].

The motivation for the work here was to investigate alternate methods to compute the exponential functions of transmutation matrices. Taylor series, Padé approximation, Chebyshev approximation, and rational Chebyshev approximation methods were compared by applying them to fuel depletion calculations. Section 2 describes these computational methods with the scaling and squaring algorithm. Section 3 presents the results of the numerical tests for one thermal reactor and two fast reactor depletion calculations. Section 4 concludes the paper.

2. Matrix Exponential Methods

In the quasi-static approximation for the burnup calculation, the nuclide transmutation equation for the nuclide density vector, $\boldsymbol{N}(t)$, at a position or burn region is represented by a system of first-order differential equations:

$$\frac{d}{dt}\boldsymbol{N}(t) = \boldsymbol{M}(\phi, \sigma, \lambda)\boldsymbol{N}(t) \qquad (1)$$

with the transmutation matrix $\boldsymbol{M}$ defined by

$$\boldsymbol{M}(\phi, \sigma, \lambda) = \langle \phi(r, E, t)\,\boldsymbol{T}(\sigma)\rangle_E + \boldsymbol{D}(\lambda) \qquad (2)$$

where $\boldsymbol{T}(\sigma)$ and $\boldsymbol{D}(\lambda)$ represent the cross section and decay matrices (including yield factors), respectively, and $\langle\ \rangle_E$ denotes the integral over energy. The formal solution of this depletion equation is obtained in terms of the exponential of the transmutation matrix as:

$$\boldsymbol{N}(t) = e^{t\boldsymbol{M}}\boldsymbol{N}_0 \qquad (3)$$

where $\boldsymbol{N}_0$ is the initial nuclide density vector.

For computing the exponential of a matrix, $e^{t\boldsymbol{M}}$, there exist dozens of methods obtained from classical results in analysis, approximation theory, and matrix theory.[5,6] These methods can be classified as series methods, ordinary differential equation methods, polynomial methods, and matrix decomposition methods. Among these various methods, Taylor or Padé approximation with a scaling and squaring algorithm is known to be one of the most effective methods.[5] Therefore, we chose the series methods with a scaling and squaring algorithm and compared their effectiveness for solving the nuclide transmutation equation.

2.1. Series Approximations

The so-called series methods for computing matrix functions are based on the idea that if a scalar function $g(z)$ approximates a scalar function $f(z)$ on the spectrum of a matrix $\boldsymbol{A}$, then $g(\boldsymbol{A})$

approximates $f(\boldsymbol{A})$. Hence, in these methods, standard approximation techniques for the scalar function e^t are directly applied to matrices. In the present work, we investigate the Taylor series, the diagonal Padé approximation, the Chebyshev approximation, and the rational Chebyshev approximation method.

In the Taylor series method, e^A is approximated through the truncation of its Taylor series as:

$$e^{A} \approx \sum_{n=0}^{k} \frac{1}{n!} \boldsymbol{A}^{n} \tag{4}$$

The order of approximation k is chosen large enough so that the truncation error is smaller than the prescribed error tolerance. In the present work, based on the inverse error analysis in Reference 5, the order k was determined as the smallest integer such that $2^{3-k} / (k+1)! \leq 10^{-8}$.

In the (p,q) Padé approximation, e^A is approximated by a rational function whose numerator and denominator are p-th and q-th order polynomials, respectively, as:

$$e^{A} \approx R_{pq}(A) = [D_{pq}(A)]^{-1} N_{pq}(A) \tag{5}$$

where

$$N_{pq}(A) = \sum_{n=0}^{p} \frac{(p+q-n)!\,p!}{(p+q)!\,n!\,(p-n)!} A^{n} \tag{6}$$

$$D_{pq}(A) = \sum_{n=0}^{q} \frac{(p+q-n)!\,q!}{(p+q)!\,n!\,(q-n)!} (-A)^{n} \tag{7}$$

Notice that $R_{p0}(\boldsymbol{A})$ is the p-th order Taylor polynomial. For a given amount of work, the diagonal approximation ($p=q$) minimizes the truncation error, and hence it is preferred over the off-diagonal approximation ($p \neq q$).[5,6] As a result, we employed the diagonal approximation $R_{qq}(\boldsymbol{A})$, and determined the order q as the smallest integer such that $2^{3-2q} (q!)^2/(2q)!\ (2q+1)! \leq 10^{-8}$ based on the inverse error analysis in Reference 5.

The Chebyshev approximation is based on the following Chebyshev series representation of the scalar function e^t in the interval [-1,1]:

$$e^{t} = I_0(1) + \sum_{n=1}^{\infty} 2I_n(1)\, T_n(t) \tag{8}$$

where T_n's are Chebyshev polynomials of the first kind and I_n's are modified Bessel functions of the first kind. If the series is truncated at the k-th order, a polynomial of degree k, whose coefficients depend on the truncation order, is obtained as:

$$e^{t} \approx \sum_{n=0}^{k} c_n(k)\, t^{n} \tag{9}$$

This polynomial is close to the minimax polynomial, which (among all polynomials of the same degree) has the smallest maximum deviation from e^t. If we apply this approximation formula to a matrix $\boldsymbol{A}$, we obtain the Chebyshev approximation formula for e^A as:

$$e^{A} \approx \sum_{n=0}^{k} c_n(k)\, \boldsymbol{A}^{n} \tag{10}$$

In this Chebyshev approximation, the approximation order k was chosen to be the same as the Taylor series approximation.

In the rational Chebyshev approximation of a scalar function e^t in the interval [-1,1], a Padé approximation is perturbed with a Chebyshev polynomial in such a way as to reduce the leading coefficient in the error $R_{pq}(t) - e^t$. This perturbation causes the error near the center of expansion to increase slightly. However, the small increase of the error near the center of expansion is compensated for by a decrease in the error farther away. If we approximate e^t by a rational function $R(t)$ with numerator of degree p and denominator of degree q and if we determine the coefficients such that the maximum absolute value of $R(t) - e^t$ for a given interval is minimized, we obtained the rational Chebyshev approximation for e^t as:

$$e^t \approx \left(\sum_{n=0}^{p} a_n t^n \right) / \left(\sum_{n=0}^{q} b_n t^n \right) \qquad (11)$$

whose coefficients depend on the degrees p and q. If we apply this approximation formula to a matrix $\boldsymbol{A}$, we obtain the rational Chebyshev approximation formula for e^A as:

$$e^A \approx \left(\sum_{n=0}^{q} b_n \boldsymbol{A}^n \right)^{-1} \left(\sum_{n=0}^{p} a_n \boldsymbol{A}^n \right) \qquad (12)$$

In the present work, we employed the diagonal approximation (i.e., $p=q$) and determined the order q to be the same as Padé approximation.

2.2. Scaling and Squaring

In a series method for computing the exponential of a matrix $t\boldsymbol{M}$, the powers of $t\boldsymbol{M}$ are added or subtracted. Hence, if two powers of $t\boldsymbol{M}$ have equally large corresponding elements, "catastrophic cancellation" occurs in the finite precision arithmetic.[7] This roundoff error difficulty generally increases as $t \| \boldsymbol{M} \|$ increases. Furthermore, in the case of Taylor and Padé approximations, the computing costs also increase as $t \| \boldsymbol{M} \|$ increases since Taylor and Padé approximants are good only near the origin.

These difficulties can be controlled by exploiting the fact that $e^{t\boldsymbol{M}} = (e^{t\boldsymbol{M}/m})^m$. Using this property of the exponential function, the matrix $t\boldsymbol{M}$ is first scaled by a power of two such that the exponential of the scaled matrix tM/m can be reliably and efficiently computed, and then the exponential of the original matrix $e^{t\boldsymbol{M}}$ is formed by repeatedly squaring the resulting matrix $e^{tM/m}$. In the present study, the scaling parameter m was chosen as the smallest power of two for which $t \| \boldsymbol{M} \|_\infty / m \le 1/2$. That is, a smallest non-negative integer J was chosen such that $2^{J-1} \ge t \| \boldsymbol{M} \|_\infty$.

3. Numerical Tests

The performance of the above four series methods was compared by applying them to local burnup calculations for an modular high temperature gas-cooled reactor (MHTGR) core[8], a 450 MWt liquid metal reactor (LMR) core[9], and the EBR-II core[10]. The burn matrices were constructed using multigroup microscopic cross section sets and the group fluxes obtained by three-dimensional nodal calculations. Nodal calculations were performed with the nodal option of the DIF3D code[11] using 10 energy groups for the MHTGR and 9 groups for the 450 MWt LMR and the EBR-II.

In the burn chains for the MHTGR problem, total 9 isotopes were employed including a lumped fission product and a dummy isotope representing a fictitious reaction end product. Since this core is designed for producing tritium using highly enriched uranium fuel and lithium target, only two heavy isotopes (U-235 and U-238) were included in the burn chains. On the other hand, Xe-135 and Sm-149 were explicitly represented because of large thermal absorption cross sections. For the 450 MWt LMR, 8 actinide isotopes (U-235, U-236, U-238, Pu-238, Pu-239, Pu-240, Pu-241, and Pu-242) were included in the burn chains, and total 12 nuclides were employed. Fission and capture reactions were considered for all 8 heavy isotopes, but (n,2n) reaction was considered only for Pu-239. The β^- decay of Pu-241 was taken into account, but the α decays of the other isotopes were neglected. The fission products were represented by three lumped fission products, and all the other end

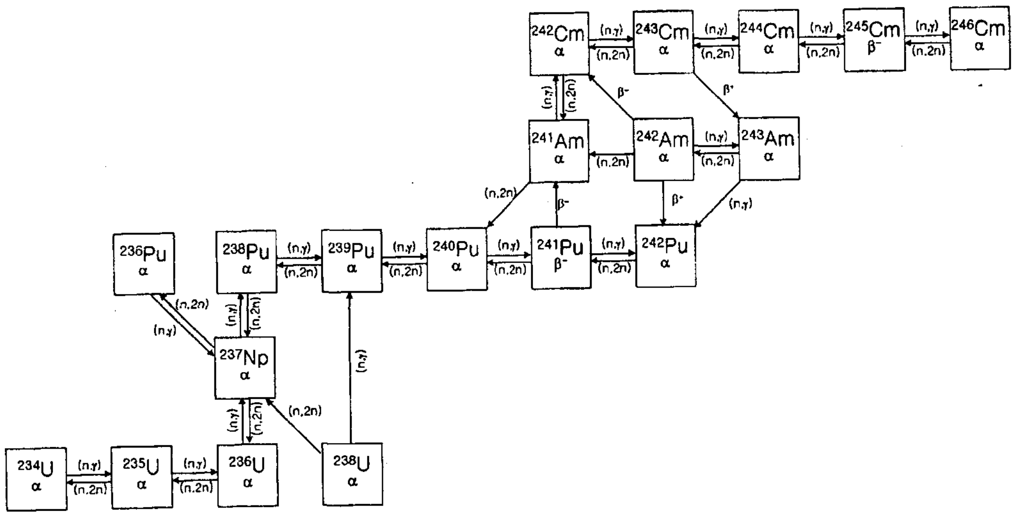

Fig. 1. Isotope Transmutation Chains Used for the EBR-II Problem

products not included in the burn chains were replaced by a dummy isotope. In the case of the EBR-II problem, more detailed burn chains were used. They were constructed using total 28 nuclides including 19 actinide isotopes from U-234 to CM-246 shown in Figure 1. Fission, capture, and (n,2n) reactions were considered for all heavy isotopes, and α and β decays were also taken into account as shown in Figure 1. Four lumped fission products were used to represent the fission products, and two burnup indicators (La-139 and Nd-148) were explicitly included. Two dummy isotopes were used to represent the other end products not included in the burn chains.

For each of these three problems, one typical burn matrix was selected, and its exponentials were computed for various burn time intervals. The infinite norms of the selected burn matrices were 6.31, 7.88×10^{-4}, and 4.64×10^{-3} for the MHTGR, the 450 MWt LMR, and the EBR-II problem, respectively. The MHTGR burn matrix has a large norm due to the large thermal cross sections. To test the accuracy of the matrix exponentials calculated with the approximate methods discussed in the previous section, reference solutions were obtained using the Taylor series approximation with the scaling and squaring algorithm. In these reference calculations, the series was summed until each element of the exponential of the scaled burn matrix converges within the machine precision. That is, we summed the series until adding another term does not alter the numbers stored in the computer.

Prior to comparing the performance of the series approximation methods, we first investigated the accuracy of the reference solutions. For this purpose, each burn matrix was decomposed based on the similarity transformation of the form $\boldsymbol{M}=\boldsymbol{X}\boldsymbol{\Lambda}\boldsymbol{X}^{-1}$, where Λ is the diagonal matrix composed of the eigenvalues of the burn matrix, and $\boldsymbol{X}$ is the matrix composed of the eigenvectors. Then the exponential functions of the burn matrix were computed as $e^{t\boldsymbol{M}}=\boldsymbol{X}e^{t\boldsymbol{\Lambda}}\boldsymbol{X}^{-1}$ for various time steps ranging from 1 day to 360 days. Compared with these exponentials, the above reference solutions showed the maximum

Table 1. Matrix Scaling Factors (as Powers of Two) and Approximation Orders

Burn Time (days)			1	50	100	150	200	250	300	360
MHTGR	Scaling Factor		4	10	11	11	12	12	12	13
	Approximation Order	Taylor	9	9	9	9	9	9	9	9
		Padé	4	4	4	4	4	4	4	4
450 MWt LMR	Scaling Factor		0	0	0	0	0	0	0	0
	Approximation Order	Taylor	9	9	9	9	9	9	9	9
		Padé	4	4	4	4	4	4	4	4
EBR-II	Scaling Factor		0	0	0	1	1	2	2	2
	Approximation Order	Taylor	9	9	9	9	9	9	9	9
		Padé	4	4	4	4	4	4	4	4

absolute difference in matrix elements less than 6.0×10^{-13} for the MHTGR, 8.9×10^{-16} for the 450 MWt LMR, and 1.2×10^{-13} for the EBR-II, while the largest element in each of these exponentials is about one. These results indicate that the matrix exponentials obtained by two independent methods are practically the same to each other. This confirms that the reference solutions determined by the converged Taylor series as described above is one of the best solutions that can be obtained with the finite precision arithmetic.

For each burn matrix, matrix exponentials were computed using Taylor, Padé, Chebyshev, and rational Chebyshev approximations, and compared with the above reference solutions. Each matrix was scaled such that its infinite norm is less than or equal to 1/2. The approximation orders of Taylor and Padé approximations were determined as described in the previous section. The approximation orders of Chebyshev approximations were the same as Taylor approximations, and those of rational Chebyshev approximations were the same as Padé approximations. Table 1 shows the matrix scaling factors as powers of two and the approximation orders for each burn time interval. The burn matrices of the 450 MWt LMR and the EBR-II have small matrix norms due to small cross sections, and hence they are nearly not scaled. On the other hand, the MHTGR burn matrix is always scaled because of the large matrix norm. As shown in Table 1, the ninth order Taylor series and the fourth order Padé series were good enough to make the estimated truncation error (based on the inverse error analysis) less than 10^{-8} when the exponential functions of the burn matrices are scaled such that their infinite norms are less than or equal to 1/2.

Figures 2 to 4 show the relative infinite norm of the error matrix in matrix exponential, i.e., the infinite norm of the difference between the approximate and the reference solution divided by the infinite norm of the reference solution. As shown in these figures, the truncation errors measured in the infinite matrix norm are smaller than 4.8×10^{-10} for all cases. This shows that the actual truncation errors are smaller than the

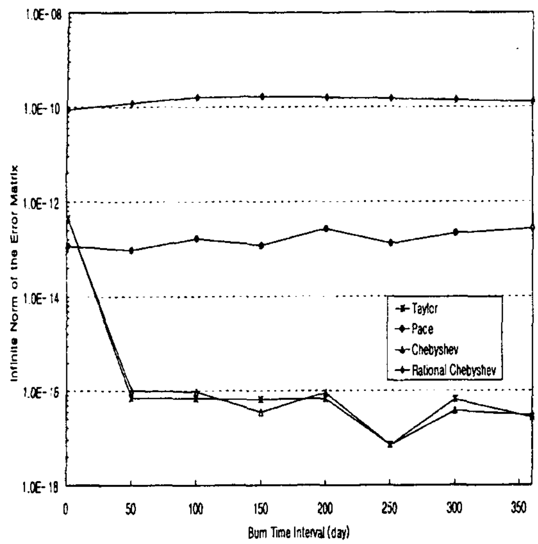

Fig. 2. Relative Infinite Norms of the Error Matrices in the Exponentials of the MHTGR Burn Matrix (Infinite Norm of the Reference Solution = 1.0)

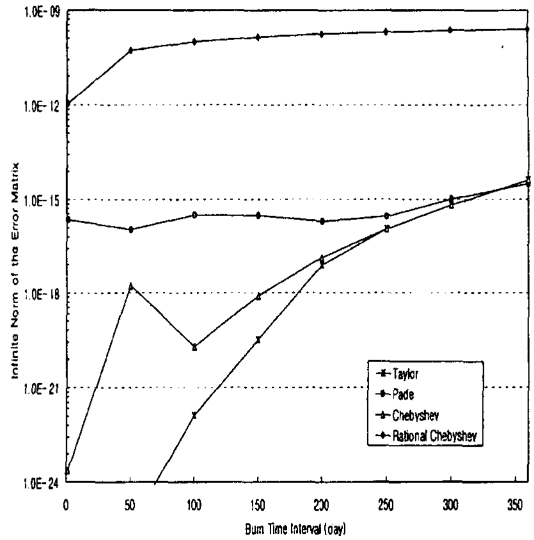

Fig. 3. Relative Infinite Norms of the Error Matrices in the Exponentials of the 450 MWt LMR Burn Matrix (Infinite Norm of the Reference Solution = 1.0)

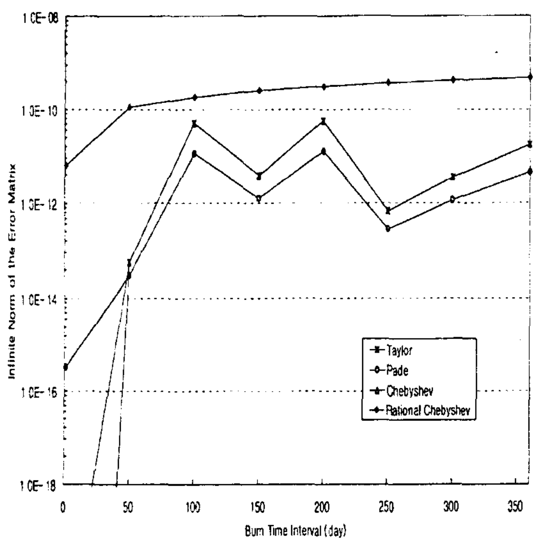

Fig. 4. Relative Infinite Norms of the Error Matrices in the Exponentials of the EBR-II Burn Matrix (Infinite Norm of the Reference Solution = 1.0)

upper bound 10^{-8} used in determining the orders of Taylor and Padé approximations. The maximum absolute errors in matrix elements are similar to the infinite norm errors shown in Figures 2 to 4, although they are slightly bigger. These results indicate that all the four series methods are accurate enough to be used for fuel depletion calculations. In each problem, the truncation error generally increases as the norm of the scaled matrix increases. This can be seen from Figures 2 to 4 and Table 1 by observing that the truncation error increases as the burn time increases unless the scaling factor is increased.

The rational Chebyshev approximation appears to be relatively less accurate than the other three methods. This seems to be due to the scaling algorithm, which makes the eigenvalues of a burn matrix clustered near the origin. On the other hand, the error of rational Chebyshev approximation is relatively insensitive to the

Table 2. Relative Computing Time of Series Methods (Reference Time = 1.0)

Burn Time (days)		1	50	100	150	200	250	300	360
MHTGR	Taylor	0.643	0.748	0.754	0.734	0.765	0.763	0.735	0.802
	Padé	0.457	0.611	0.626	0.603	0.639	0.640	0.614	0.680
	Chebyshev	0.610	0.751	0.756	0.728	0.764	0.765	0.734	0.804
	Rational Chebyshev	0.448	0.610	0.625	0.598	0.636	0.636	0.611	0.675
450 MWt LMR	Taylor	0.874	0.765	0.701	0.649	0.649	0.603	0.604	0.605
	Padé	0.520	0.471	0.454	0.404	0.399	0.372	0.372	0.373
	Chebyshev	0.839	0.765	0.703	0.650	0.655	0.603	0.604	0.608
	Rational Chebyshev	0.513	0.467	0.429	0.397	0.398	0.369	0.369	0.371
EBR-II	Taylor	0.514	0.418	0.399	0.423	0.424	0.466	0.445	0.447
	Padé	0.294	0.240	0.229	0.260	0.260	0.303	0.290	0.290
	Chebyshev	0.509	0.416	0.397	0.421	0.422	0.464	0.443	0.444
	Rational Chebyshev	0.292	0.239	0.230	0.261	0.260	0.301	0.289	0.289

magnitude of the matrix norm. The Chebyshev approximation shows error behaviors similar to the Taylor series. Compared to Taylor or Chebyshev approximation, Padé approximation shows similar errors for the 450 MWt LMR and EBR-II problems, but bigger errors for the MHTGR problem. It is considered that the relatively bigger error of Padé approximation for the MHTGR problem results from the error introduced in the inverse of the denominator due to the roundoff errors, since the transmutation matrix has relatively widely spread eigenvalues.

Table 2 shows the computing times of four series methods relative to the reference computing time as a function of burn time interval. The reference solutions take more time as the burn time interval increases. The computing time of the reference solution also increases more rapidly as the matrix size is getting bigger, i.e., more nuclides are included in the burn chains. In the aspect of the computational efficiency, the Chebyshev approximation is similar to the Taylor series, while the rational Chebyshev approximation is similar to the Padé approximation. As shown in Table 2, the rational approximations are ~ 1.7 times faster than the polynomial approximations for the LMR problems whose burn matrices have small matrix norms. In the case of the MHTGR burn matrix whose norm is relatively large, the rational approximation is ~ 1.2 times faster than the polynomial approximations.

4. Conclusion

Series expansion methods to compute the exponential of a matrix were compared by applying them to fuel depletion calculations. Specifically, Taylor, Padé, Chebyshev, and rational Chebyshev approximations were investigated by approximating the exponentials of burn matrices by truncated series of each method. The scaling and squaring algorithm was also employed in order to avoid the catastrophic cancellation occurring in the finite precision arithmetic and to reduce the computing costs.

The computational accuracy and efficiency of these methods were tested by performing various numerical tests using one thermal reactor and two fast reactor depletion problems. In order to test the accuracy, the reference solutions were obtained by the converged Taylor series method with the scaling and squaring algorithm. The accuracy of the reference solutions was also tested by comparing them with the exponential functions determined by the similarity transformation method.

The results indicate that all the four series methods are accurate enough to be used for fuel depletion calculations although the rational Chebyshev approximation is relatively less accurate. They also show that the rational approximations are more efficient than the polynomial approximations. Considering the computational accuracy and efficiency, the Padé approximation appears to be better than the other methods investigated in this study. Its accuracy is better than that of the rational Chebyshev approximation, while being comparable to Taylor series or Chebyshev approximation. On the other hand, its efficiency is similar to that of the rational Chebyshev approximation and is better than Taylor series or Chebyshev approximation. In particular, for LMR depletion calculations, it is faster than Taylor series or Chebyshev approximation by a factor of ~ 1.7.

Acknowledgement

This work was supported by the Korea Science and Engineering Foundation through the Center for Advanced Reactor Research at Korea Advanced Institute of Science and Technology.

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