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Generalization of the analytical inversion method for the solution of the point kinetics equations

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Abstract

A method based on the analytical inversion of polynomials of the point kinetics matrix is applied to the solution of the reactor kinetics equations. This method permits a fast inversion of polynomials by going temporarily to the complex plane. Several cases using various options of the method are presented for comparison. The method developed was found to be very fast and accurate, and has the ability to reproduce all the features of transients, including prompt jump. The analysis of the assumption of constant parameters, reactivity, and source, during a time step, are included. It is concluded that the method provides a fast and accurate computational technique for the point kinetics equations with step reactivity.

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1. Introduction

In the model considered here, the point reactor kinetics equations are a system of coupled linear ordinary differential equations. Included in that system are equations which describe the neutron level, reactivity, an arbitrary number of delayed neutron groups, and any other variables that enter into the reactivity equation. There are many ways in which solutions have been obtained for the point kinetics equations. If the equations have constant coefficients, exact analytical solutions are easily established, but they are elusive when the coefficients vary with time. A time-dependent reactivity inserted into a point reactor is coupled multiplicatively with the neutron density to form a set of linear equations with time-dependent coefficients. This time dependence makes it difficult to obtain an analytical solution and numerical integration is usually employed [1–4]. However, the stiffness of the point kinetics equations restricts the time step to a small increment, making the numerical solution very inefficient.

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Several methods have been proposed to overcome this difficulty, but they do not seem fully satisfactory because of their lack of accuracy, generality, and/or simplicity. In some of these methods a generalized point kinetics formulation results, in which the elements of the ordinary point kinetics equations are replaced by matrices having a similar, but more generalized, physical meaning [5].

In what follows, we propose to apply another method, which is not only expected to be very fast and accurate, but also has the ability to reproduce all the features of transients, including prompt jump, which is not very well represented in some of the other methods. This method is based on a generalization of the analytical procedures for inverting polynomials in the point kinetics matrix, which has been included in the solution of the point kinetics equations. Also, an approximate expression for the exponential function that was suggested by a scheme called the 'purification method' [6] is introduced.

This paper is organized as follows. The formulation of the point kinetics equations in matrix form and the general approximate form of the exponential functions are summarized in section 2. The generalization of the analytical inversion method for inverting the point kinetics matrix is introduced in section 3. An analysis of the assumption of constant parameters is sketched in section 4. Section 5 describes numerical results for different approximate expressions, options, and times. Finally, conclusions are presented in section 6.

2. Method of solution

The space kinetics equations for G delayed groups are given in terms of the generation time [7] as

$$\frac{dN(t)}{dt} = \frac{\rho(t) - \beta}{\Lambda} N(t) + \sum_{i=1}^G \lambda_i C_i(t) + F(t) \quad (1)$$

$$\frac{dC_i(t)}{dt} = \frac{\beta_i}{\Lambda} N(t) - \lambda_i C_i(t) \quad i = 1, 2, \dots, G \quad (2)$$

where $N(t)$ is the neutron density, $C_i(t)$ is the precursor density, $\rho(t)$ is the time-dependent reactivity, β_i is the i th delayed fraction, $\beta = \sum_i \beta_i$ is the total delayed fraction, Λ is the generation time, λ_i is the i th-group decay constant, and G is the total number of delayed neutron groups.

The quantities $N(t)$, $C_i(t)$, $F(t)$, and $\rho(t)$ are, in general, functions of the time t ; and β_i , λ_i , and Λ are assumed constant. In addition, $\rho(t)$ may be a function of $N(t)$ in feedback problems.

We define the $G + 1$ -dimensional column vector $\Psi(t)$ as follows:

$$\Psi(t) = \text{col}[N(t) \ C_1(t) \ \dots \ C_G(t)].$$

Also, we define the matrix \mathbf{A} as the $G + 1 \times G + 1$ matrix

$$\mathbf{A}(t) = \begin{pmatrix} \frac{\rho(t) - \beta}{\Lambda} & \lambda_1 & \lambda_2 & \dots & \lambda_G \\ \frac{\beta_1}{\Lambda} & -\lambda_1 & 0 & \dots & 0 \\ \frac{\beta_2}{\Lambda} & 0 & -\lambda_2 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{\beta_G}{\Lambda} & 0 & 0 & \dots & -\lambda_G \end{pmatrix}.$$

Equations (1) and (2) can be written in matrix form as:

$$\frac{d\boldsymbol{\Psi}(t)}{dt} = \mathbf{A}(t)\boldsymbol{\Psi}(t) + \mathbf{F}(t) \quad (3)$$

where $\mathbf{F}(t)$ is the source term defined as

$$\mathbf{F}(t) = \text{col}[F(t) \ 0 \ \dots \ 0].$$

The matrix $\mathbf{A}(t)$ is usually called the point kinetics matrix, where ρ and F vary with time. Equation (3) is usually solved in a series of time steps, the assumption being that ρ and F are constant and equal to their average values during the time step under consideration. It is shown that this assumption yields a local error of the order of the cube of the time step size. The implications of this assumption are analysed later, in section 4.

The exact solution of equation (3) under the assumption of constant A is given by

$$\boldsymbol{\Psi}_{n+1}(t) = \exp(h\mathbf{A})\boldsymbol{\Psi}_n(t) + \mathbf{A}^{-1}[\exp(h\mathbf{A}) - \mathbf{I}]\mathbf{F}(t) \quad (4)$$

where h is the step time interval, $h = t_{n+1} - t_n$, $n = 0, 1, 2, 3, \dots$, $\boldsymbol{\Psi}_n$ is the value of the vector $\boldsymbol{\Psi}$ at time t_n , and $\boldsymbol{\Psi}_{n+1}$ is the value of the vector $\boldsymbol{\Psi}$ at time t_{n+1} .

Note that the last term of equation (4), a matrix term multiplying \mathbf{F} , is always well defined even if the point kinetics matrix \mathbf{A} is singular.

The mathematical treatment of the system of equation (4) is a relatively simple one; its solution can be found in practice by calculating all the eigenvalues of the matrix \mathbf{A} and performing straightforward computations. However, this is an expensive scheme, especially when the reactivity varies with time, since the calculation of the eigenvalues amounts to solving a $(G + 1)$ th-order algebraic equation (the inhour formula) for all its roots at every time step.

The eigenvectors of \mathbf{A} , denoted by \mathbf{U}_n , and the corresponding eigenvalues denoted by ω_n , obey the relation

$$\mathbf{A}\mathbf{U}_n = \omega_n\mathbf{U}_n.$$

The values of ω_n are the roots of the inhour formula

$$\rho = \omega\Lambda + \omega \sum_{i=1}^G \frac{\beta_i}{\lambda_i + \omega}.$$

It is well known that the eigenvalues, ω_n , are distinct; hence the eigenvectors, \mathbf{U}_n , are complete.

In the following section, the method of determining a general approximate expression of the exponential function for the point kinetics equations will be summarized. First let us introduce the following fact: for any function $f(\mathbf{A})$ for which $f(\omega_i)$ is bounded for all i , the following expression [6]:

$$\exp(\mathbf{A}) = f(\mathbf{A}) + \sum_{i=0}^G [\exp(\omega_i) - f(\omega_i)]\mathbf{U}_i\mathbf{V}_i^T \quad (5)$$

holds for any matrix \mathbf{A} satisfying

$$\mathbf{A}\mathbf{U}_i = \omega_i\mathbf{U}_i \quad \text{and} \quad \mathbf{A}^T\mathbf{V}_i = \omega_i\mathbf{V}_i$$

where $\mathbf{U}_i^T\mathbf{V}_i = 1$ —i.e. normalized to unity.

Since two matrices with the same eigenvalues and eigenvectors are identical, equation (5) is true if we arrive using this equation at the relation

$$\exp(\mathbf{A})\mathbf{U}_k = \exp(\omega_k)\mathbf{U}_k \quad \text{for all } \mathbf{U}_k.$$

But $\mathbf{V}_i^T\mathbf{U}_k = \delta_{ik}$, since the eigenvalues of the matrix \mathbf{A} and of \mathbf{A}^T form a biorthonormal set when properly normalized [8]. Thus, having both sides of equation (5) act on \mathbf{U}_k :

$$\begin{aligned} \exp(\mathbf{A})\mathbf{U}_k &= f(\omega_k)\mathbf{U}_k + \sum_{i=0}^G [\exp(\omega_i) - f(\omega_i)]\mathbf{U}_i\delta_{ik} \\ &= f(\omega_k)\mathbf{U}_k + [\exp(\omega_k) - f(\omega_k)]\mathbf{U}_k = \exp(\omega_k)\mathbf{U}_k. \end{aligned} \quad (6)$$

To suit our particular needs we introduce the factor h . Equation (5) then becomes

$$\exp(h\mathbf{A}) = f(h\mathbf{A}) + \sum_{i=0}^G [\exp(h\omega_i) - f(h\omega_i)]\mathbf{U}_i\mathbf{V}_i^T \quad (7)$$

where \mathbf{U}_i and \mathbf{V}_i are the unchanged eigenvectors of the matrices \mathbf{A} and \mathbf{A}^T respectively since

$$(h\mathbf{A})\mathbf{U}_i = (h\omega_i)\mathbf{U}_i \quad \text{and} \quad (h\mathbf{A}^T)\mathbf{V}_i = (h\omega_i)\mathbf{V}_i.$$

Equation (7) has a form that permits us to approximate $\exp(h\mathbf{A})$ in an economical fashion. It is interesting to note that, if $f(h\omega_i)$ is a good approximation for $\exp(h\omega_i)$, then we are justified in dropping the i th term from the summation. It will have a very small coefficient:

$$[\exp(h\omega_i) - f(h\omega_i)] \ll 1. \quad (8)$$

Since $\exp(h\omega_i) \approx f(h\omega_i)$, to a high degree of accuracy, we have

$$\exp(h\mathbf{A}) \approx g(h\mathbf{A}) = f(h\mathbf{A}) + \sum_k' [\exp(h\omega_k) - f(h\omega_k)]\mathbf{U}_k\mathbf{V}_k^T \quad (9)$$

where the sum \sum_k' is over only those k for which equation (8) does not hold.

Equation (7) is, so far, a mere result of mathematical manipulation. It has, however, a form that permits us to approximate $\exp(h\mathbf{A})$ in an economical manner. The vectors \mathbf{U}_k and \mathbf{V}_k are easily calculated from their defining equation:

$$\{\omega\mathbf{I} - \mathbf{A}\}\mathbf{U}_k = 0 \quad \text{so} \quad \mathbf{U}_k = \text{col} \left[1 \quad \frac{\mu_1}{\lambda_1 + \omega_k} \quad \cdots \quad \frac{\mu_G}{\lambda_G + \omega_k} \right].$$

Similarly for \mathbf{V}_k :

$$\{\omega\mathbf{I} - \mathbf{A}^T\}\mathbf{V}_k = 0 \quad \text{so} \quad \mathbf{V}_k = \text{col} \left[1 \quad \frac{\lambda_1}{(\lambda_1 + \omega_k)} \quad \cdots \quad \frac{\lambda_G}{(\lambda_G + \omega_k)} \right]$$

or, in the normalized form:

$$\mathbf{V}_k = v_k \text{col} \left[1 \quad \frac{\lambda_1}{(\lambda_1 + \omega_k)} \quad \cdots \quad \frac{\lambda_G}{(\lambda_G + \omega_k)} \right]$$

where v_k is the normalization factor—which satisfies the normalization condition $\mathbf{U}_i^T\mathbf{V}_i = 1$ —given by

$$v_k = \left[1 + \sum_{i=1}^G \frac{\mu_i\lambda_i}{(\lambda_i + \omega_k)^2} \right]^{-1} < 1.$$

3. Analysis of the analytical inversion

For an arbitrary matrix \mathbf{X} , the power series

$$\mathbf{I} + \mathbf{X} + \frac{\mathbf{X}^2}{2!} + \frac{\mathbf{X}^3}{3!} + \cdots \quad (10)$$

converges to a matrix which is called the exponential of \mathbf{X} (Taylor's series expansion), and which is denoted by $\exp(\mathbf{X})$. Direct appeal to the series definition, expression (10), is impractical [9], since the number of computations needed for each additional term makes the computing time prohibitive. In view of this and to avoid the instabilities associated with the computational effort involved in using the explicit methods, equation (9) requires a particular class of approximation for the exponential function.

The Padé rational approximations and related inversions. Here we consider a particular class of approximations for the exponential functions, namely the Padé rational approximations [10]. These approximations are known to be consistent and unconditionally stable when the numerator is a polynomial of the same degree as the denominator or smaller. For any of these approximations in which the degree of the polynomial's denominator is larger than unity, we have a full square matrix of order $(G + 1)$ to invert. That is a task that one normally tries to avoid, particularly for the case of varying reactivity where such inversion needs to be done at every time step. To avoid the above difficulty and to save time in calculations, we have developed a method in which by going temporarily to the complex plane, we obtain simple analytical expressions for such inverses. As a result, the computational effort involved in using implicit methods of any order is equal to that required in explicit methods of the same order (Taylor series expansions). However, the instabilities associated with the latter are avoided.

The method developed is based on an expression for the inverse of $[\mathbf{I} - \varepsilon \mathbf{X}]$ where ε is a scalar complex number. When one tries to invert a general polynomial in the matrix \mathbf{X} , which can be expressed as a product of factors having the form $[\mathbf{I} - \varepsilon \mathbf{X}]$, the utility of the method developed is evident, in general, for any matrix polynomial $P_k(\mathbf{X})$. To see this utility in more detail, consider the following matrix polynomial:

$$P_k(\mathbf{X}) = \sum_{n=0}^k C_n \mathbf{X}^n$$

with C_n being a real number and $C_0 = 1$.

The matrix polynomial $P_k(\mathbf{X})$ can be factored as

$$P_k(\mathbf{X}) = \prod_{n=1}^k [\mathbf{I} - \varepsilon_n \mathbf{X}]$$

where ε_n are, in general, complex numbers; then,

$$[P_k(\mathbf{X})]^{-1} = \prod_{n=1}^k [\mathbf{I} - \varepsilon_n \mathbf{X}]^{-1}.$$

The constants ε_n will either be real numbers or form complex conjugate pairs.

The method of factorization considered above is of great advantage and has direct applicability to the Padé approximations used later as approximations to the exponential matrix, equation (9).

Analytical inversion. In this section the analytical inversion method is applied to the point kinetic matrix \mathbf{A} . As we mentioned above, the method is based on an expression for the inverse of $[\mathbf{I} - \varepsilon \mathbf{A}]$; thus for a real ε the following expression is introduced:

$$[\mathbf{I} - \varepsilon \mathbf{A}]^{-1} = \gamma^{-1} \mathbf{B} + \mathbf{C} \quad (11)$$

where

$$\gamma = \left[1 - \frac{\varepsilon \rho}{\Lambda} + \varepsilon \sum_{i=1}^G \frac{\mu_i}{1 + \varepsilon \lambda_i} \right],$$

$$\mathbf{C} = \text{Diag} \left[0, \frac{1}{1 + \varepsilon \lambda_1}, \frac{1}{1 + \varepsilon \lambda_2}, \frac{1}{1 + \varepsilon \lambda_3}, \dots, \frac{1}{1 + \varepsilon \lambda_G} \right],$$

$$\mathbf{B} = \mathbf{a} \mathbf{b}^T$$

and

$$\mathbf{a} = \text{col} \begin{bmatrix} 1 & \frac{\varepsilon\mu_1}{1+\varepsilon\lambda_1} & \frac{\varepsilon\mu_2}{1+\varepsilon\lambda_2} & \cdots & \frac{\varepsilon\mu_G}{1+\varepsilon\lambda_G} \end{bmatrix}$$

$$\mathbf{b} = \text{col} \begin{bmatrix} 1 & \frac{\varepsilon\lambda_1}{1+\varepsilon\lambda_1} & \frac{\varepsilon\lambda_2}{1+\varepsilon\lambda_2} & \cdots & \frac{\varepsilon\lambda_G}{1+\varepsilon\lambda_G} \end{bmatrix}.$$

G is the number in the delayed neutron group, which is considered here as a 6-group. Equation (11) is easily coded when γ is a scalar that depends on the reactivity.

Similarly, we can define

$$[\mathbf{I} - \bar{\varepsilon}\mathbf{A}]^{-1} = \bar{\gamma}^{(-1)}\mathbf{D} + \mathbf{E}$$

where $\bar{\gamma}$, \mathbf{D} , and \mathbf{E} are the complex conjugates of γ , \mathbf{B} , and \mathbf{E} respectively.

Expression (11) is of no great advantage by itself, since we can solve the system of equations implied by the inverse shown directly with essentially the same computational effort as is required in this case. However, the utility of the analytical inversion is evident when the ε_n form a complex conjugate pair. In this case the following pairing of factors:

$$[\mathbf{I} - \varepsilon\mathbf{A}]^{-1}[\mathbf{I} - \bar{\varepsilon}\mathbf{A}]^{-1} = [\mathbf{I} - 2\text{Re}(\varepsilon)\mathbf{A} + |\varepsilon|^2\mathbf{A}^2]^{-1}$$

is considered, which is a real matrix and thus has a real inverse. This expression can be expressed in general form as

$$[\mathbf{I} - \varepsilon\mathbf{A}]^{-1}[\mathbf{I} - \bar{\varepsilon}\mathbf{A}]^{-1} = \gamma^{-1}\bar{\gamma}^{(-1)}\mathbf{B}\mathbf{D} + \gamma^{-1}\mathbf{B}\mathbf{E} + \bar{\gamma}^{(-1)}\mathbf{C}\mathbf{D} + \mathbf{C}\mathbf{E}$$

$$= (\gamma\bar{\gamma})^{-1}\mathbf{F} + \gamma^{-1}\mathbf{G} + \bar{\gamma}^{(-1)}\mathbf{H} + \mathbf{Q}. \quad (12)$$

For generality, assume that $\varepsilon = a + ib$ and $\bar{\varepsilon} = a - ib$, where a and b are real constants and $i = \sqrt{-1}$, so we have

$$\gamma\bar{\gamma} = 1 - \frac{2a\rho}{\Lambda} + \left(\frac{r\rho}{\Lambda}\right)^2 + \sum_{i=1}^G 2\mu_i P_i (a + r^2\lambda_i) - \frac{r^2\rho}{\Lambda} \sum_{i=1}^G 2\mu_i P_i (1 + a\lambda_i)$$

$$+ r^2 \left(\sum_{i=1}^G \mu_i P_i\right)^2 + 2ar^2 \left(\sum_{i=1}^G \mu_i P_i\right) \left(\sum_{i=1}^G \mu_i P_i \lambda_i\right) + r^4 \left(\sum_{i=1}^G \mu_i P_i \lambda_i\right)^2$$

where

$$r^2 = a^2 + b^2 \quad \text{and} \quad P_i^{-1} = (1 + 2a\lambda_i + r^2\lambda_i^2), \quad i = 1, \dots, G.$$

The \mathbf{F} can be written in terms of its elements as $\mathbf{F} = \mathbf{B}\mathbf{D} = [f_{k\ell}]$, where

$$f_{11} = 1 + \sum_{i=1}^G r^2 \mu_i \lambda_i P_i \quad f_{1\ell+1} = \frac{\bar{\varepsilon}\lambda_\ell}{(1 + \bar{\varepsilon}\lambda_\ell)} f_{11} \quad \ell = 1, 2, \dots, G$$

$$f_{k+1\ 1} = \frac{\varepsilon\mu_k}{(1 + \varepsilon\lambda_k)} f_{11} \quad f_{k+1\ \ell+1} = \frac{r^2 \mu_k \lambda_\ell}{(1 + \varepsilon\lambda_k)(1 + \bar{\varepsilon}\lambda_\ell)} f_{11} \quad k = 1, 2, \dots, G.$$

The matrix \mathbf{G} is defined in terms of its elements as $\mathbf{G} = \mathbf{B}\mathbf{E} = [g_{kl}]$, where $g_{11} = 0$, and

$$g_{1\ell+1} = \varepsilon\lambda_\ell P_\ell \quad g_{k+1\ 1} = 0 \quad g_{k+1\ \ell+1} = \frac{\varepsilon^2 \mu_k \lambda_\ell}{(1 + \varepsilon\lambda_k)} P_\ell.$$

The matrix \mathbf{H} , the product of the matrices \mathbf{C} and \mathbf{D} , is defined in terms of its elements as $\mathbf{H} = \mathbf{C}\mathbf{D} = [h_{k\ell}]$, where

$$h_{11} = 0 \quad h_{1\ell+1} = 0 \quad h_{k+1\ 1} = \bar{\varepsilon}\mu_k P_k \quad h_{k+1\ \ell+1} = \frac{\bar{\varepsilon}^2 \mu_k \lambda_\ell}{(1 + \bar{\varepsilon}\lambda_\ell)} P_k.$$

Finally, the matrix $\mathbf{Q} = \mathbf{CE} = [q_{k\ell}]$ is the diagonal matrix where $q_{\ell+1 \ell+1} = P_\ell$; otherwise $q_{k\ell} = 0$.

Expression (12) can be rewritten as

$$[\mathbf{I} - \varepsilon\mathbf{A}]^{-1}[\mathbf{I} - \bar{\varepsilon}\mathbf{A}]^{-1} = (\gamma\bar{\gamma})^{(-1)}\mathbf{FF} + \mathbf{Q} \tag{13}$$

where the matrix \mathbf{FF} is the combination of the above-defined matrices:

$$\mathbf{FF} = \mathbf{F} + \bar{\gamma}\mathbf{G} + \gamma\mathbf{H} = [ff_{k\ell}].$$

Almost all of the elements involved can be precomputed since only the reactivity changes with time, and it appears in a simple fashion in the coefficients of the dyads as shown later in a specific example.

Applications on the Padé approximations using analytical inversion. As we mentioned before, equation (7) or its equivalent form equation (9) requires a particular class of approximations for the exponential function, called the Padé rational approximations. These approximations can be written in general as $f_{mk}(\mathbf{A}) = P_m(\mathbf{A})/Q_k(\mathbf{A})$ where $P_m(\mathbf{A})$ and $Q_k(\mathbf{A})$ are polynomials of degree m and k , respectively [10]. We shall call $N = m + k$ the index of $f_{mk}(\mathbf{A})$. We note the important fact that, among all the desired Padé approximations, those for $m = k$ or $k + 1$ give the smallest (minimum maximum) error for a given N . For any of these approximations for which the degree of the polynomial's denominator, $Q_k(\mathbf{A})$, is larger than unity, we have a full square matrix of order $(G + 1)$ to invert using the method adopted.

As an example, four implicit rational functions are studied in this work (see equation (7)):

$$f_1(\varepsilon\mathbf{A}) = [\mathbf{I} - \varepsilon\mathbf{A}]^{-1} \tag{14}$$

$$f_2(\varepsilon\mathbf{A}) = [\mathbf{I} - \varepsilon\mathbf{A}]^{-1}[\mathbf{I} + \varepsilon\mathbf{A}] \tag{15}$$

$$f_3(\varepsilon\mathbf{A}) = [\mathbf{I} - \varepsilon\mathbf{A}]^{-1}[\mathbf{I} - \bar{\varepsilon}\mathbf{A}]^{-1} \tag{16}$$

$$f_4(\varepsilon\mathbf{A}) = [\mathbf{I} - \varepsilon\mathbf{A}]^{-1}[\mathbf{I} - \bar{\varepsilon}\mathbf{A}]^{-1}\left[\mathbf{I} + \frac{h}{3}\mathbf{A}\right] \tag{17}$$

corresponding, respectively, to the Padé (0, 1), Padé (1, 1), Padé (0, 2) and Padé (1, 2) approximations of the exponential [11]. The corresponding factors of the complex constant ε are $h(1, 0)$, $(h/2)(1, 0)$, $(h/2)(1 + i)$ and $(h/3)(1 + \frac{1}{\sqrt{2}}i)$ respectively with $i = \sqrt{-1}$. Using equation (11) and carrying out some involved but straightforward algebra, all imaginary numbers in the final expression will be eliminated.

In the following sections, a discussion will be given of two representative reactors, the thermal and fast reactors. The values for Λ , β_i , and λ_i (in s^{-1}) for these reactors are shown in table 1, for six delayed neutron groups.

3.1. Padé (0, 1) approximation

The first approximation, equation (14), involves no particular difficulties except that one always has to choose h such that $h\omega_i \neq 1$ to keep $f(h\omega_i)$ bounded. Since only the ω_0 -eigenvalue of \mathbf{A} can be positive, we must have $h\omega_0 \neq 1$. For small h the error of this approximation is given by

$$\exp(h\mathbf{A}) - f_1(h\mathbf{A}) = -\frac{h^2\mathbf{A}^2}{2} + O(h^3).$$

This approximation is the explicit version for equation (11) with $\varepsilon = h$. Since all eigenvalues of \mathbf{A} have small magnitudes except possibly ω_5 , ω_6 , and ω_0 , these will be the only ones to be calculated explicitly (see table 2) for use in equation (9), if we do not

Table 1. Parameters for two typical reactors.

Neutron group	Thermal reactor		Fast reactor	
	λ_i	β_i	λ_i	β_i
1	0.0127	2.8500E-04	0.0129	1.6720E-04
2	0.0317	1.5975E-03	0.0311	1.2320E-03
3	0.115	1.4100E-03	0.134	9.5040E-04
4	0.311	3.0525E-03	0.331	1.4430E-03
5	1.40	9.6000E-04	1.260	4.5340E-04
6	3.87	1.9500E-04	3.210	1.5400E-04
		$\beta_{tot} = 0.007500$	$\beta_{tot} = 0.0044$	
		$\Lambda = 5.0E-04$ s	$\Lambda = 1.0E-07$ s	

want to take a very small h -value. In the case of a thermal reactor within the time interval $0.1 \text{ s} \leq h \leq 1.0 \text{ s}$, we have, hence: $3.211 \times 10^{-2} \leq |\exp(h\omega_6) - f_1(h\omega_6)| \leq 0.203$ for ω_6 and $0.041 \leq |\exp(h\omega_5) - f_1(h\omega_5)| \leq 0.204$ for ω_5 , which correspond to $h\omega_6 \leq -0.438$ and $h\omega_5 \leq -0.248$ within the reactivity interval $(-1\$, +1\$)$. A feature shared by the following cases is that the effect of the ω_0 -term rapidly increases with increasing reactivity, which indicates that the effect of the ω_0 -term should be included in equation (9), where $1.5 \times 10^{-4} \leq |\exp(h\omega_0) - f_1(h\omega_0)| \leq 0.716$ for both reactors. On the other hand, in the case of a fast reactor it is enough to require the inclusion of ω_k -terms in equation (9), simply by making $h\omega_i$ ($i = 1, 2, \dots, 6$) less than -0.292 , to include explicit treatment of negative ω_i . In fact, these values are low enough to require the inclusion of the most effective ω_k -terms in equation (9) only when $h\omega_i \leq 0.688$. The above considerations, coupled with the fact that for most practical cases only one of ω_0 and ω_k is of large magnitude, indicate that in many problems, satisfactory results will be obtained by treating explicitly more than one term in equation (9); table 2 confirms this fact.

3.2. Padé (1, 1) approximation

This approximation, represented by equation (15), is valid for any real values of $h\omega_i$, except that one must always choose h such that $h\omega_i \neq 2$. For small h the error of this approximation is given by

$$\exp(h\mathbf{A}) - f_2(h\mathbf{A}) = -\frac{h^3\mathbf{A}^3}{12} + O(h^4).$$

The method developed, equation (11), is directly applied to find the inverse of the first term in $f_2(h\mathbf{A})$ with $a = h/2$ and $b = 0$, so $\varepsilon = h(1 + 0i)/2$.

The results for this case are in general similar to the previous ones; in the case of a thermal reactor, as we mentioned above, all the eigenvalues of the matrix \mathbf{A} have small magnitude except possibly ω_0 , ω_5 , and ω_6 . The values of the coefficient for negative ω_i are within the interval $(2.83 \times 10^{-10}, 0.87)$, while they are within the interval $(0.0, 0.036)$ for positive values of ω_i (table 2); these cases correspond to $h\omega_i \leq -0.248$ and $h\omega_0 \leq 0.608$ respectively (equation (8)). On the other hand, for a fast reactor it is enough to take the value of $h\omega_i$ less than 0.688 to cover the explicit treatment for both the extreme values of ω_i -terms. From the above discussion, the inclusion of ω_i -terms in equation (9) will occur only when $h\omega_i \leq 0.688$, which is the same condition as in the previous case.

Table 2. Values of the coefficients $[\exp(h\omega_i) - f(h\omega_i)]$ for different cases of Padé approximations. ω_i ($i = 1, 2, 3, 4$), $\omega_0, \omega_5, \omega_6$ are the real roots of the inhour equation. (1\$ \equiv 1 dollar of reactivity.)

Type	Reactivity	ω	Case 1 $\exp(h\omega_i) - f_1(h\omega_i)$		Case 2 $\exp(h\omega_i) - f_2(h\omega_i)$		Case 3 $\exp(h\omega_i) - f_3(h\omega_i)$		Case 4 $\exp(h\omega_i) - f_4(h\omega_i)$		
			min	max	min	max	min	max	min	max	
Thermal reactor	-1\$	ω_0	0.0	7.224E-5	0.0	1.474E-7	0.0	2.921E-7	0.0	5.344E-10	
		ω_i	1.129E-6	1.632E-1	2.833E-10	6.150E-2	5.660E-10	4.589E-2	3.735E-11	8.965E-3	
	0\$	ω_5	4.005E-2	1.869E-1	3.088E-3	3.343E-1	4.615E-3	6.132E-2	1.734E-4	6.757E-2	
		ω_6	3.202E-2	2.033E-1	8.522E-2	8.759E-1	2.049E-3	6.899E-2	1.360E-2	9.830E-2	
	0\$	ω_0	0.0	7.163E-1	0.0	3.691E-2	0.0	1.034E-1	0.0	4.210E-3	
		ω_i	8.584E-7	1.560E-1	1.878E-10	1.669E-2	3.753E-10	4.248E-2	3.256E-11	7.536E-3	
	1\$	ω_5	2.086E-2	2.036E-1	9.954E-4	3.283E-1	1.645E-3	6.879E-2	3.830E-5	6.638E-2	
		ω_6	5.020E-2	2.025E-1	4.656E-3	7.711E-1	6.622E-3	6.863E-2	2.997E-4	9.830E-2	
	Fast reactor	-(3/4)\$	ω_0	0.0	7.115E-5	0.0	1.440E-7	0.0	2.855E-7	0.0	5.236E-10
			ω_i	1.091E-6	1.524E-1	2.692E-10	5.031E-2	5.378E-10	4.084E-2	3.672E-11	6.918E-3
		0\$	ω_5	3.006E-2	1.987E-1	1.861E-3	2.661E-1	2.926E-3	6.718E-2	8.828E-5	5.337E-2
			ω_6	1.299E-5	2.272E-4	9.991E-1	9.999E-1	3.373E-10	1.033E-7	2.597E-5	4.538E-4
0\$		ω_0	0.0	1.545E-2	0.0	5.906E-2	0.0	1.672E-1	0.0	7.655E-3	
		ω_i	8.970E-7	1.478E-1	2.006E-10	4.625E-2	4.009E-10	3.879E-2	3.328E-11	6.204E-3	
(3/4)\$		ω_5	2.719E-2	2.012E-1	1.564E-3	2.618E-1	2.496E-3	6.828E-2	7.000E-5	5.242E-2	
		ω_6	2.273E-5	9.081E-4	9.964E-1	9.999E-1	1.033E-9	1.649E-6	4.545E-5	1.806E-3	

3.3. The Padé (0, 2) approximation

Equation (16) represents the second-order implicit approximation Padé (0, 2). This approximation is commonly valid for any real value of $h\omega_i$; for small h -values the error of this approximation is given by

$$\exp(h\mathbf{A}) - f_3(h\mathbf{A}) = \frac{h^3\mathbf{A}^3}{6} + O(h^4).$$

This approximation is applied directly to equation (12) to find the inverse of $f_3(h\mathbf{A})$, where $\varepsilon = h(1+i)/2$.

It should be noted that only the scalar $\gamma\bar{\gamma}^{-1}$ depends on the reactivity and therefore everything can be precomputed. For this approximation we have $5.66 \times 10^{-10} \leq |\exp(h\omega_i) - f_3(h\omega_i)| \leq 0.069$ for all negative ω_i -values (maximum 0.069 at $h\omega_i = -2.65$) within the reactivity interval $(-1, +1)$ in both thermal and fast reactors (table 2). This figure is small enough that a result of high accuracy can be obtained by treating explicitly only the ω_0 -term in equation (9). Moreover, if $|h\omega_0|$ is sufficiently below unity, as in the case of a thermal reactor, none of the ω_k -terms in equation (9) needs to be considered explicitly.

3.4. The Padé (1, 2) approximation

This approximation is called the Padé (1, 2) and is given in the equivalent form

$$f_4(h\mathbf{A}) = \left[\mathbf{I} - \frac{2}{3}h\mathbf{A} + \frac{h^2\mathbf{A}^2}{6} \right]^{-1} \left[\mathbf{I} + \frac{h\mathbf{A}}{3} \right] \quad (18)$$

where $f_4(h\mathbf{A}) \neq 0$ for any real value of $h\omega_i$. An explicit application of the method developed will be used here to find the inverse of the first term in $f_4(h\mathbf{A})$. Using the complex factorization method, equation (17) can be rewritten in the equivalent form of equation (18) where $a = h/3$ and $b = h/3\sqrt{2}$; for small h , the error of this approximation is given by

$$\exp(h\mathbf{A}) - f_4(h\mathbf{A}) = -\frac{5}{54}h^3\mathbf{A}^3 + O(h^4).$$

In the case of thermal and fast reactors, we have for this approximation $0.0 \leq |\exp(h\omega_i) - f_4(h\omega_i)| \leq 0.0983$ for all negative ω_i -values (maximum 0.0982 at $h\omega_i = -8.49$), while for positive values of ω_i we have $0.0 \leq |\exp(h\omega_i) - f_4(h\omega_i)| \leq 0.0077$ within the same range of reactivity (table 2). This analysis shows that results of high accuracy can be obtained by treating explicitly just ω_0 -, ω_5 -, and ω_6 -terms for the extreme values of reactivity in a thermal reactor. Moreover, in the case of a fast reactor, if $h\omega_0$ is sufficiently below unity, none of the ω_k -terms in equation (9) needs to be considered explicitly.

4. Analysis of the assumption

The complex factorization method used above could be applied to the denominator of any higher order of Padé approximation. The following section reveals that there is no advantage in going beyond $O(h^3)$, since there is an $O(h^3)$ error inherent in the assumption of constant reactivity and source during the same time step as will be shown here.

The local discretization error gives an idea of the error incurred when the exact solution Ψ_{n+1}^{exact} is used in place of the approximate solution Ψ_{n+1}^{app} due to the assumption of constant reactivity and source during a time step. Taking them equal to their average values during a time interval h yields the smallest error. This is the error of the approximate solution after one

time step, under the assumption that no error existed at the beginning. The components of the true solution Ψ_{n+1}^{exact} are first expanded in a Taylor's series about the point t as

$$\Psi_{n+1}^{exact}(t) = \Psi_n(t) + h\dot{\Psi}_n(t) + \frac{h^2}{2!}\ddot{\Psi}_n(t) + \frac{h^3}{3!}\dddot{\Psi}_n(t) + \dots \quad (19)$$

With repeated use of $\dot{\Psi}_n = \mathbf{A}_n\Psi_n + \mathbf{F}_n$, equation (19) becomes

$$\begin{aligned} \Psi_{n+1}^{exact} = & \left[\mathbf{I} + h\mathbf{A}_n + \frac{h^2}{2!}(\mathbf{A}_n^2 + \dot{\mathbf{A}}_n) + \frac{h^3}{3!}(\mathbf{A}_n^3 + 2\dot{\mathbf{A}}_n\mathbf{A}_n + \mathbf{A}_n\dot{\mathbf{A}}_n + \ddot{\mathbf{A}}_n) + \dots \right] \Psi_n \\ & + \left[h\mathbf{F}_n + \frac{h^2}{2!}(\dot{\mathbf{F}}_n + \mathbf{A}_n\mathbf{F}_n) + \frac{h^3}{3!}(\ddot{\mathbf{F}}_n + \mathbf{A}_n\dot{\mathbf{F}}_n + 2\dot{\mathbf{A}}_n\mathbf{F}_n + \mathbf{A}_n^2\mathbf{F}_n) + \dots \right]. \end{aligned} \quad (20)$$

By taking the average value of the parameters in equation (4) over the time step, the following solution is obtained:

$$\Psi_{n+1}^{app} = \exp(h\bar{\mathbf{A}})\bar{\Psi}_n + \bar{\mathbf{A}}^{-1}[\exp(h\bar{\mathbf{A}}) - \mathbf{I}]\bar{\mathbf{F}}.$$

Taylor's series expansion for $\exp(h\bar{\mathbf{A}})$ gives

$$\Psi_{n+1}^{app} = \left[\mathbf{I} + h\bar{\mathbf{A}} + \frac{h^2}{2!}\bar{\mathbf{A}}^2 + \frac{h^3}{3!}\bar{\mathbf{A}}^3 + \dots \right] \bar{\Psi}_n + h \left[\mathbf{I} + \frac{h}{2!}\bar{\mathbf{A}} + \frac{h^2}{3!}\bar{\mathbf{A}}^2 + \dots \right] \bar{\mathbf{F}} \quad (21)$$

where

$$\bar{\mathbf{A}} = \frac{1}{h} \int_{t_n}^{t_{n+1}} \mathbf{A}(t) dt = \mathbf{A}_n + \frac{h}{2!}\dot{\mathbf{A}}_n + \frac{h^2}{3!}\ddot{\mathbf{A}}_n + \dots$$

and

$$\bar{\mathbf{F}} = \frac{1}{h} \int_{t_n}^{t_{n+1}} \mathbf{F}(t) dt = \mathbf{F}_n + \frac{h}{2!}\dot{\mathbf{F}}_n + \frac{h^2}{3!}\ddot{\mathbf{F}}_n + \dots$$

Substituting these expansions into equation (21) gives

$$\begin{aligned} \Psi_{n+1}^{app} = & \left[\mathbf{I} + h\mathbf{A}_n + \frac{h^2}{2!}(\mathbf{A}_n^2 + \dot{\mathbf{A}}_n) + \frac{h^3}{3!}(\mathbf{A}_n^3 + \frac{3}{2}\dot{\mathbf{A}}_n\mathbf{A}_n + \ddot{\mathbf{A}}_n) + \dots \right] \bar{\Psi}_n \\ & + \left[h\mathbf{F}_n + \frac{h^2}{2!}(\dot{\mathbf{F}}_n + \mathbf{A}_n\mathbf{F}_n) + \frac{h^3}{3!}(\ddot{\mathbf{F}}_n + \frac{3}{2}\mathbf{A}_n\dot{\mathbf{F}}_n + \frac{3}{2}\dot{\mathbf{A}}_n\mathbf{F}_n + \mathbf{A}_n^2\mathbf{F}_n) + \dots \right]. \end{aligned} \quad (22)$$

Subtracting equation (22) from equation (20) and assuming that $\Psi_n = \bar{\Psi}_n$, it is seen that

$$\Psi_n^{exact} - \Psi_n^{app} = \frac{h^3}{12}(\dot{\mathbf{A}}_n\mathbf{A}_n - \mathbf{A}_n\dot{\mathbf{A}}_n)\Psi_n + \frac{h^3}{12}(\dot{\mathbf{A}}_n\mathbf{F}_n - \mathbf{A}_n\dot{\mathbf{F}}_n) + O(h^4). \quad (23)$$

In other words the local discretization error of the method defined by equation (4) is of the order $O(h^4)$. Thus it may be expected that the global error of the method is $O(h^3)$. It should be noted that expression (23) still holds if $\mathbf{A}(t)$ and $\mathbf{F}(t)$ are known only through a three-term Taylor's expansion, which requires only knowledge of \mathbf{A} , \mathbf{F} , and their first and second derivatives at the beginning of the time step.

5. Numerical results

Six different transients are considered here, all starting from the equilibrium conditions and with $N(0) = 1$. In each case the source term is taken to be zero. The algorithm is coded (figure 1) for different cases and all the calculations are done on an IBM Pentium II 300 MHz

Table 3. The RPE values of the exact $N(t)$ and the method developed compared with Gauss elimination method (11).

h	Case	$t = 0.1$ s	$t = 1.0$ s	$t = 10$ s
0.001	a	-1.8392E-04	-4.6259E-04	-1.8764E-03
	b	2.4046E-04	1.7768E-03	1.6154E-02
	c	3.5063E-04	1.7779E-03	1.6155E-02
0.01	a	-3.8719E-05	-2.9267E-05	-2.0530E-04
	b	-3.4660E-05	7.9574E-05	1.2548E-03
	c	1.0991E-02	1.8334E-04	1.2985E-03
0.1	a	-3.9055E-05	1.1515E-05	-3.7179E-05
	b	-3.8519E-05	2.3780E-05	1.1760E-04
	c	1.2025E+00	9.9495E-03	4.4864E-03
0.25	a		-2.2062E-05	-9.6936E-05
	b	—	-1.2544E-05	-9.0806E-05
	c		5.1292E-02	2.7231E-02
0.5	a		-9.9295E-05	-1.1623E-04
	b	—	-1.0030E-04	-1.0503E-04
	c		-3.7412E+00	1.0932E-01
1.0	a		-7.2831E-04	-2.5981E-04
	b	—	-7.3157E-04	-2.7175E-04
	c		2.0267E+01	3.9539E-01
Exact $N(t)$		1.533 113	2.511 494	14.215 03

^a The analytical inversion with explicit treatment of the roots.

^b The Gauss elimination with explicit treatment of the roots.

^c The Gauss elimination without explicit treatment of the roots.

computer using Visual FORTRAN compilations. The relative percentage errors (RPEs) of the calculations are defined as follows:

$$\text{RPE} = \left(\frac{N_{\text{calc}} - N_{\text{exact}}}{N_{\text{exact}}} \right) \%$$

where N_{exact} is obtained using the explicit equation (20) and involving a small time step, with the assumption of constant reactivity and source during the time.

The method developed is compared in table 3 with the conventional method, the Gauss elimination method [11], used to invert the polynomial of the point kinetic matrix and the reactor response as well. The results correspond to a step reactivity insertion of +0.5\$ in a thermal reactor. The calculations are done by three methods: (a) the analytical inversion method which permits a fast inversion of a polynomial with automatic treatment of the roots; (b) the Gauss elimination method, also with automatic treatment of the roots; and (c) the Gauss elimination method with no explicit treatment of the roots. The results for the RPEs in table 3 show parallel behaviour for methods (a) and (b) at all the transient points. However, the RPE in method (a) is the best for most of the transient points. A deviation in the range from 10^{-1} to 10^{-4} for method (c) is recorded compared with those of the other methods.

Tables 4–7 shows the exact results based on the explicit method, equation (10) with a very small time step, and the RPEs of the calculations for the several options of the method adopted in this work.

The results for selected times t during the transient and for several values of the time step size h used in the calculations are shown within the reactivity interval ($-1\$, +1\%$) for the selected reactors. The results for both thermal and fast reactors are shown in figure 2 at large time and in figure 3 at small time; all the computations started from initial equilibrium with $N(0) \equiv 1$ neutron/cm³.

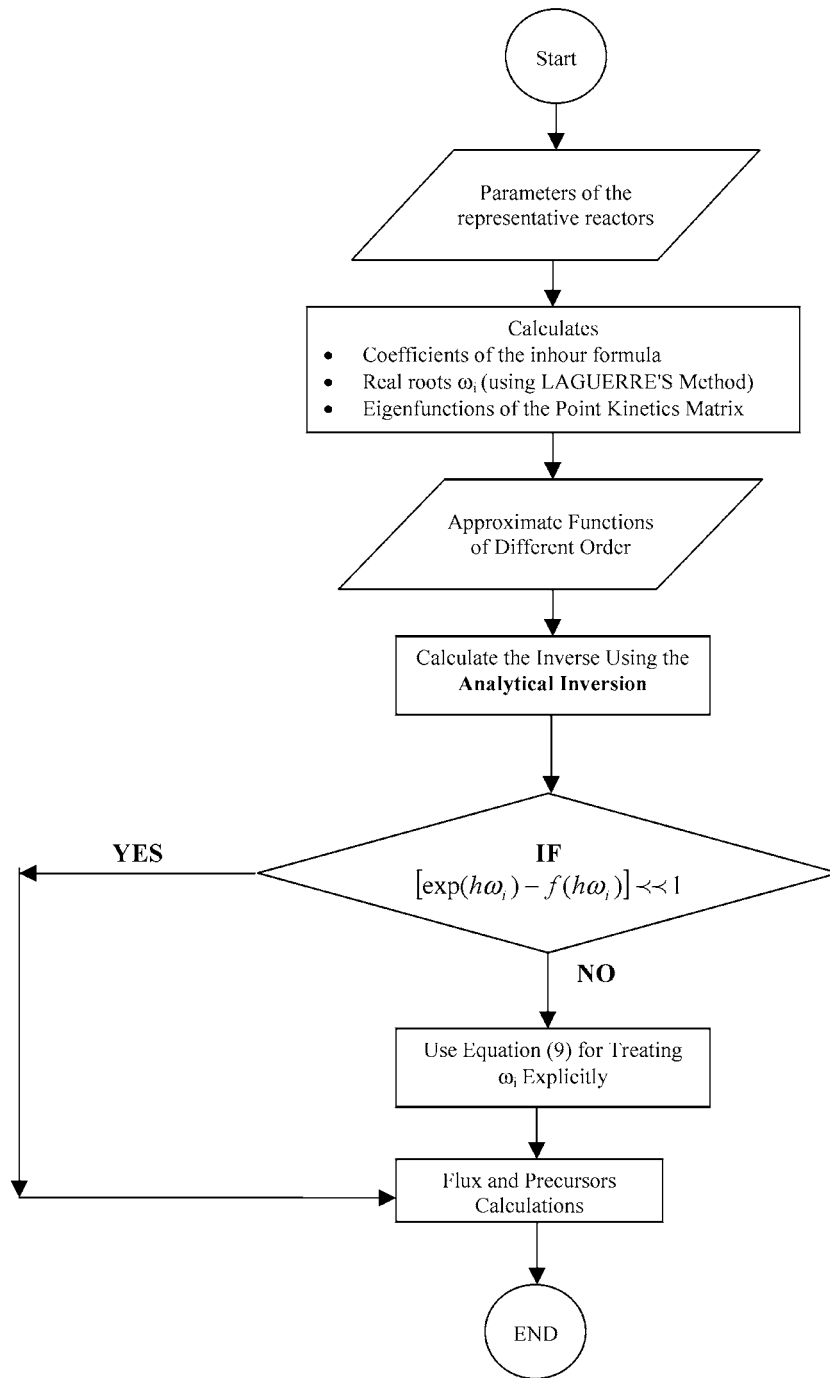


Figure 1. Block diagram for the method of calculation.

The numbers in each section are in exponential notation and correspond to the method described for each case that follows. As an example of numerical results, these cases will be summarized for a few points of reactivity to be discussed later. Four cases are considered here

Table 4. The RPEs and exact $N(t)$ for case 1.

h	Case	$t = 0.1$ s	$t = 1.0$ s	$t = 10$ s
0.001	a	-2.0925E-05	1.6918E-05	-2.4293E-05
	b	-1.8392E-04	-4.6259E-04	-1.8764E-03
	c	-2.0261E-04	-5.1714E-04	-2.0873E-03
	d	-3.2964E-04	-8.9222E-04	-3.5376E-03
	e	-7.9441E-02	-7.5010E-04	-1.5077E-02
0.01	a	-2.3272E-06	4.1130E-05	3.6649E-05
	b	-3.8719E-05	-2.9267E-05	-2.0530E-04
	c	-4.3647E-05	-4.4038E-05	-2.6218E-04
	d	-4.6292E-05	-4.8771E-05	-2.8247E-04
	e	-7.6836E-01	-7.8501E-03	-1.5131E-01
0.1	a	1.1905E-04	8.7174E-05	2.5109E-06
	b	-3.9055E-05	1.1515E-05	-3.7179E-05
	c	-1.2029E-05	5.7285E-07	-1.1716E-04
	d	-3.2525E-05	-6.0222E-06	-1.0677E-04
	e	-5.8750E+00	-1.0758E-01	1.5391E+00
0.25	a	—	1.1328E-04	4.3163E-05
	b	—	-2.2062E-05	-9.6936E-05
	c	—	7.9370E-05	7.4881E-05
	d	—	1.8614E-05	-1.7235E-05
	e	—	-4.1137E-01	3.9631E+00
0.5	a	—	3.1431E-05	-1.4087E-05
	b	—	-9.9295E-05	-1.1623E-04
	c	—	7.3602E-05	-3.7176E-05
	d	—	4.9712E-06	-1.0877E-05
	e	—	-1.2039E+00	8.3419E+00
1.0	a	—	-8.3037E-05	-5.4203E-05
	b	—	-7.2831E-04	-2.5981E-04
	c	—	3.1258E-05	-1.4379E-04
	d	—	-1.5878E-04	-1.2936E-04
	e	—	-3.0368E+00	1.8634E+01
Exact $N(t)$		1.533 113	2.511 494	14.215 03

^a Corresponds to Padé (0, 1) with automatic inclusion of ω_i -terms.

^b Corresponds to Padé (1, 1) with automatic inclusion of ω_i -terms.

^c Corresponds to Padé (0, 2) with automatic inclusion of ω_i -terms.

^d Corresponds to Padé (1, 2) with automatic inclusion of ω_i -terms.

^e Corresponds to Padé (0, 1) without automatic inclusion of ω_i -terms.

and the calculations are done using four methods: (i) Padé (0, 1); (ii) Padé (1, 1); (iii) Padé (0, 2); and (iv) Padé (1, 2).

Case 1. This case corresponds to a positive ramp insertion of reactivity of +0.5\$ in a thermal reactor (table 4). The calculations are done using the above four methods with the automatic inclusion of ω_i -terms, mainly ω_0 -, ω_5 -, and ω_6 -terms. By automatic inclusion of both ω_0 - and ω_6 -terms, we mean that these roots are treated explicitly whenever the terms $h\omega_0$ and $h\omega_6$ are larger than a certain value. Otherwise, ω_0 - and ω_6 -terms are not included. The last row in each section introduces RPEs for the method (i) without inclusion of ω_i -terms.

Generally, the results for this case show that the RPEs for the first four methods are quite small (less than $1.0 \times 10^{-4}\%$) for h as large as 1.0 s, while for the first method it is quite large without explicit treatment of the roots.

Table 5. The RPEs and exact $N(t)$ for case 2.

h	Case	$t = 0.1$ s	$t = 1.0$ s	$t = 10$ s
0.001	a	6.6342E-06	1.3879E-06	4.0946E-06
	b	-7.6947E-05	-1.0096E-04	-1.6361E-04
	c	-6.8315E-06	-1.5193E-05	-2.2939E-05
	d	-2.4545E-04	-3.0748E-04	-5.0170E-04
	e	-5.4589E-04	-1.0133E-04	-1.6365E-04
0.01	a	1.1528E-05	7.5368E-06	1.4479E-05
	b	-8.2233E-07	-8.2001E-06	-9.9665E-06
	c	1.6025E-05	1.2387E-05	2.3603E-05
	d	7.9911E-06	2.1637E-06	7.7652E-06
	e	-4.7029E-02	-4.5130E-05	-1.3564E-05
0.1	a	6.2576E-06	-2.9558E-06	-6.5858E-06
	b	1.0940E-05	-4.3318E-08	4.7399E-06
	c	1.3916E-06	6.7033E-08	-2.4196E-06
	d	3.6189E-06	-3.6406E-06	-2.9868E-06
	e	-7.7845E+00	-3.6968E-03	-3.5667E-04
0.25	a	—	-3.3476E-05	-3.8453E-05
	b	—	-1.7341E-05	-1.0513E-05
	c	—	2.0046E-05	2.0988E-05
	d	—	4.6811E-06	1.2242E-05
	e	—	2.8264E+00	-2.2662E-03
0.5	a	—	-8.2509E-05	-9.0215E-05
	b	—	-4.4657E-05	-2.6079E-05
	c	—	6.0808E-07	-1.5642E-05
	d	—	-5.6934E-06	2.3732E-06
	e	—	2.6186E+01	5.9246E-02
1.0	a	—	-1.1357E-04	-1.1605E-04
	b	—	-2.0040E-06	-4.1472E-05
	c	—	-3.7405E-05	-7.7836E-05
	d	—	-9.7169E-06	-2.0362E-05
	e	—	-4.5462E+01	1.4065E+01
Exact $N(t)$		0.698 9252	0.607 0536	0.396 0777

^a Corresponds to Padé (0, 1) with automatic inclusion of ω_i -terms.

^b Corresponds to Padé (1, 1) with automatic inclusion of ω_i -terms.

^c Corresponds to Padé (0, 2) with automatic inclusion of ω_i -terms.

^d Corresponds to Padé (1, 2) with automatic inclusion of ω_i -terms.

^e Corresponds to Padé (1, 1) without automatic inclusion of ω_i -terms.

Comparison of the first row in each section in table 4 with the last row of the same section shows a large correction effect obtained by treating ω_0 -, ω_5 -, and ω_6 -terms explicitly, a feature shared by some of the other following cases.

Case 2. This case considers the results for a thermal reactor in which a -0.5% step reactivity is inserted. Table 5 shows the results for this case. Calculations are done using the same four methods as were mentioned for case 1 and compared with method (ii) without explicit treatment of the roots.

Again, in this case the RPEs for the methods considered are approximately of the same order of magnitude. Although the RPEs for the treated and untreated methods (method (ii)) are of the same order of magnitude at some points of the transient, the errors of the other methods treated are nevertheless also quite small. The transient is very accurately represented by the above four methods due to the explicit treatment of the most dominant roots, in this case ω_0 , ω_5 , and ω_6 , which is documented by the results obtained.

Table 6. The RPEs and exact $N(t)$ for case 3.

h	Case	$t = 0.1$ s	$t = 1.0$ s	$t = 10$ s
0.001	a	1.9282E-05	8.4159E-06	4.2151E-05
	b	4.3973E-06	-1.2127E-05	-2.0617E-05
	c	-5.7893E-06	-1.1585E-05	-2.6421E-05
	d	1.4800E-05	1.2208E-06	1.3275E-05
	e	7.4893E-06	-8.4848E-06	-1.7080E-05
0.01	a	2.8300E-05	2.0406E-05	7.6443E-05
	b	3.3043E-06	-1.4631E-05	-3.3020E-05
	c	1.1099E-05	-5.0423E-06	-9.9471E-06
	d	1.8805E-05	4.4877E-06	1.2174E-05
	e	-4.0172E+01	-6.1113E+00	1.8320E-06
0.1	a	2.8751E-05	2.2004E-05	8.3209E-05
	b	-6.6887E-06	-1.8272E-05	-3.7868E-05
	c	9.9437E-06	-5.9627E-06	-9.9781E-06
	d	1.1792E-05	-3.3672E-06	-2.5568E-06
	e	4.8099E+01	-3.6967E+01	-6.5374E+00
0.25	a	—	4.0780E-06	1.9430E-05
	b	—	-1.6303E-05	-3.4070E-05
	c	—	2.8805E-05	1.0629E-04
	d	—	-2.1708E-05	-5.5819E-05
	e	—	-3.7514E+01	-7.6004E+00
0.5	a	—	1.4461E-05	5.6928E-05
	b	—	-3.8110E-08	6.6703E-06
	c	—	-2.8372E-05	-8.7621E-05
	d	—	1.6460E-06	8.9460E-06
	e	—	-3.7616E+01	-7.7102E+00
1.0	a	—	-1.6932E-05	-5.5530E-05
	b	—	1.1561E-05	2.8143E-05
	c	—	-1.2868E-05	-3.6749E-05
	d	—	-2.4082E-05	-6.2240E-05
	e	—	3.8331E+01	-7.5186E+00
Exact $N(t)$		2.075 317	2.655 853	12.746 54

^a Corresponds to Padé (0, 1) with automatic inclusion of ω_i -terms.

^b Corresponds to Padé (1, 1) with automatic inclusion of ω_i -terms.

^c Corresponds to Padé (0, 2) with automatic inclusion of ω_i -terms.

^d Corresponds to Padé (1, 2) with automatic inclusion of ω_i -terms.

^e Corresponds to Padé (0, 2) without automatic inclusion of ω_i -terms.

Case 3. The results of this case are shown in table 6, and correspond to a step reactivity insertion of +0.5\$ in a fast reactor. Calculations are done using the same four methods as mentioned above and compared both with each other and with method (iii) without explicit treatment of the roots. In this example, the most effective part arises from treating explicitly ω_4 - and ω_5 -terms, while the effects of the other ω_i -terms are negligible.

Again, the errors for the four methods are of the same order of magnitude, which means that there are parallel behaviours for the four methods in this case. At small transient time ($t = 0.001$ s) the RPE results from method (iii) without treating the roots explicitly are considered valuable if compared with the other methods. In contrast, at large transient time ($t \geq 0.01$) the RPEs are very large as compared with those of the other methods. The results for the method with untreated roots are in general not accepted except for small h .

Table 7. The RPEs and exact $N(t)$ for case 4.

h	Case	$t = 0.1$ s	$t = 1.0$ s	$t = 10$ s
0.001	a	-6.0654E-07	-4.4717E-06	4.5911E-06
	b	-3.6011E-06	-7.8965E-06	-6.4343E-07
	c	-4.9612E-06	-9.5020E-06	-3.3001E-06
	d	-1.9756E-06	-6.2540E-06	6.6580E-07
	e	-2.0273E-06	-6.4194E-06	-6.9699E-08
0.01	a	2.3805E-06	-5.7690E-07	1.1906E-05
	b	-1.0647E-05	-1.5082E-05	-8.6354E-06
	c	-3.1133E-06	-6.9771E-06	1.9170E-06
	d	-1.8824E-06	-5.5237E-06	3.8023E-06
	e	-2.0305E-06	-5.8388E-06	2.8908E-06
0.1	a	2.3627E-06	-28491E-07	1.1366E-05
	b	-4.7339E-06	-1.1329E-05	-4.4730E-06
	c	-3.5705E-06	-7.6548E-06	1.6914E-07
	d	-1.1996E-06	-5.2347E-06	2.6493E-06
	e	-1.5426E-02	-9.4280E-05	8.9608E-07
0.25	a	—	-4.1403E-06	5.3978E-06
	b	—	-1.1742E-05	-4.6462E-06
	c	—	1.3766E-06	1.4466E-05
	d	—	-9.5557E-06	-3.0760E-06
	e	—	-1.2994E-03	-1.9589E-05
0.5	a	—	-1.3888E-06	9.7116E-06
	b	—	-7.6456E-06	8.6293E-07
	c	—	-1.2961E-05	-7.8950E-06
	d	—	-4.3319E-06	4.3048E-06
	e	—	-9.5459E-03	-1.2189E-04
1.0	a	—	-9.2281E-06	-1.3519E-06
	b	—	-8.5505E-06	2.7237E-06
	c	—	-9.1955E-06	-1.7689E-06
	d	—	-1.1871E-05	-6.4360E-06
	e	—	-8.5030E-02	-9.8362E-06
Exact $N(t)$		0.658 5039	0.608 4439	0.419 7024

- ^a Corresponds to Padé (0, 1) with automatic inclusion of ω_i -terms.
- ^b Corresponds to Padé (1, 1) with automatic inclusion of ω_i -terms.
- ^c Corresponds to Padé (0, 2) with automatic inclusion of ω_i -terms.
- ^d Corresponds to Padé (1, 2) with automatic inclusion of ω_i -terms.
- ^e Corresponds to Padé (1, 2) without automatic inclusion of ω_i -terms.

Table 8. The CPU time of calculations for the different methods. All the calculations were done under the same conditions.

Method	CPU time step (s 10^{-4})
Padé (0, 1)	4.47
Padé (1, 1)	5.13
Padé (0, 2)	4.74
Padé (1, 2)	6.06
Reference	4.85

Case 4. This final case corresponds to a step reactivity of -0.5% in a fast reactor (table 7). The calculations are done using the same four methods, and they are compared with those

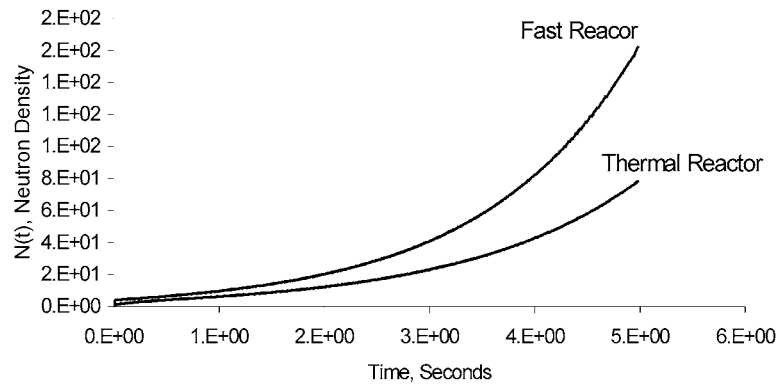


Figure 2. Reactor response to a step reactivity change of $3/4\%$.

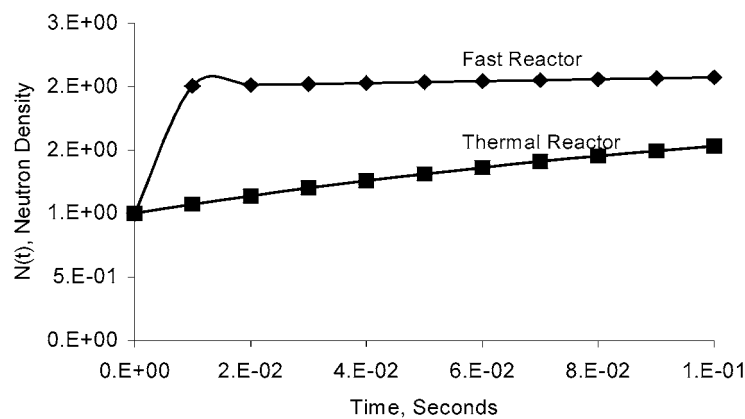


Figure 3. Reactor response to a step reactivity change of $1/2\%$ at small time.

from method (iv) without treating the roots explicitly. The resulting RPEs are approximately of the same order of magnitude for all methods at small transient times, while the error becomes relatively large at large transient time steps. The most effective part in this case comes from the ω_5 -term, while a small effect arises from the ω_6 -term. By automatic inclusion of ω_5 , we mean that this root is treated explicitly whenever $h\omega_5$ is larger than a certain value, which is less than or equal to -0.292 in this case. The best results are obtained in this case for small transient times for the method with untreated roots, but this is purely accidental, since method (iv) with treatment of the roots is an improvement over the same method without treatment of the roots.

6. Conclusions

An analytical inversion method is developed to permit a fast inversion of polynomials in the point kinetics matrix and with direct applicability to the Padé approximations represented by equations (14)–(17).

The method, for most purposes, adequately solves the reactor kinetics equations for many options and times. Numerical examples of applying the method to a variety of problems confirmed that the time step size can be greatly increased and that much computing time can be saved, as compared with other conventional methods. The CPU time required for

the analytical inversion of the point kinetics matrix \mathbf{A} is less than the time required for the conventional method (Gauss elimination) by 77.64%. Also, table 4 showed that the accuracy at all transient points compares excellently with another conventional method, which means that the method developed is of general validity and involves no effective approximations. The results in tables 3–7 showed the greatest improvement over the Padé approximation with the explicit treatment of the most dominant effective roots. This improvement is reflected not only in the achievement of great accuracy at all time steps, but also in the ability to use large time steps without incurring large errors.

Table 8 shows the CPU time for the calculations for different types of Padé approximation compared with the reference calculations. This comparison shows the dependence of the CPU time on the number of arithmetic operations for the different cases. However, the relative times for the calculations for the different types of approximation are found to be 1 : 1.15 : 1.06 : 1.36 : 1.08 for Padé (0, 1), Padé (1, 1), Padé (0, 2), Padé (1, 2), and the reference calculation (table 8).

Generally, the RPEs of the above-mentioned treated methods for most options and times are very small and approximately of the same order of magnitude (tables 3–7). Also, treating the roots of the inhour formula would make the Padé approximation inaccurate or yield large errors.

Calculations for the other points of reactivity were made (data not shown) and they confirmed the conclusions, which reflect the general validity and agree with theoretical expectations. The method developed is particularly good for cases in which the reactivity can be represented by a series of steps and performs quite well for more general cases.

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