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ACCELERATION OF THE OUTER ITERATIONS OF THE SPACE-DEPENDENT NEUTRON KINETICS EQUATIONS SOLUTION

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Abstract - A variant of the Chebyshev iterative procedure, called the Chebyshev Semi-Analytical (CSA) method, is developed for acceleration of outer iterations of the space-dependent neutron kinetics equations solution. A Chebyshev polynomials sequence is chosen to optimize the convergence of residual vectors to the eigenvector of the iteration matrix. When the convergence is attained, the "exact" solution is computed by adding an error vector to the obtained approximate solution. Convergence rate of the CSA method is determined by the second eigenvalue of the iteration matrix in contrast to the Chebyshev Semi-Iterative (CSI) method where it is defined by the spectral radius of the same matrix. An adaptive Chebyshev procedure is modified for estimation of the optimum iteration parameters of the CSA method.

The proposed method is implemented in the 3D neutron kinetics computer code SKETCH. The numerical results of benchmark problem calculations demonstrate that the CSA method is 2-5 times faster than the CSI method for delayed critical transient calculations. The relative effectiveness of the CSA method increases with increase in time step size.

I. INTRODUCTION

Nuclear reactor core analysis demands accurate and sufficiently fast computer codes for transient calculations. A three-dimensional computer code SKETCH has been developed initially as a neutronics part of the integrated neutronics/thermohydraulics computer code for the analysis of advanced fast nuclear reactor dynamics (Schukin et. al., 1993). First results of the neutron kinetics benchmark problems calculations (Schukin et. al., 1994) indicated that the computer code SKETCH could also be applied to light water reactor analysis. The mathematical model of the code is based on few-group space-dependent neutron kinetics equations in diffusion approximation. The mesh-centered finite-difference method is used for spatial approximation of the equation set in X-Y-Z and triangular-Z geometry. The obtained time-dependent equations are discretized by using a fully-implicit scheme to the neutron flux equations in combination with a "time-integrated" approximation to the delayed neutron precursors equations (Stacey, 1969). The discretized equations are solved iteratively at each time step using a standard combination of outer and inner iterations. The convergence of unaccelerated outer iterations is very slow for practical neutron kinetics problems and therefore the computational efficiency of the code depends significantly on the utilised acceleration technique.

This paper presents the iterative procedure that has been developed for the acceleration of the outer iterations in the SKETCH code. The procedure, called the Chebyshev Semi-Analytical (CSA)

method, is based on an application of the Chebyshev polynomials and analytical refinement of the iterative approximation by adding the error vector to the obtained solution. In Section II of this paper, the finite-difference form of the neutron kinetics equations is presented. The Fission Source Iteration (FSI) method and the previously developed Modified Fission Source Iteration (MFSI) method (Zimin and Schukin, 1992) based on the Aitken extrapolation step (Fox, 1964) are considered in Section III. Chebyshev acceleration of the FSI method and the MFSI method that result in the traditional Chebyshev Semi-Iterative (CSI) method and the proposed Chebyshev Semi-Analytical method respectively are discussed in Section IV. Determination of the optimum iteration parameters for the CSA method requires the estimation of a second eigenvalue of the iteration matrix. A priori and adaptive procedures to compute this eigenvalue are discussed in Section V. During transient calculations information from the previous time step can be taken into account in order to obtain an "optimal" initial approximation. The "optimal" initial approximation for the CSA and MFSI methods that results in the initial residual vector which is close to the first eigenvector of the iteration matrix is presented in Section VI. The influence of the inner iterations method on the convergence properties of the outer iterations is considered in Section VII. A comparison of the CSI, MFSI and CSA methods for two neutron kinetics benchmark problems is given in Section VIII. Section IX concludes the discussions of the paper.

II. NEUTRON KINETICS EQUATIONS

The few-group neutron kinetics equations can be written as

$$\frac{1}{V_g}\frac{\partial \varphi_g(\mathbf{r},t)}{\partial t} = \nabla D_g(\mathbf{r},t)\nabla\varphi_g(\mathbf{r},t) + \Sigma_g^r(\mathbf{r},t)\varphi_g(\mathbf{r},t) - \sum_{g'\neq g}\Sigma_{gg'}^s(\mathbf{r},t)\varphi_{g'}(\mathbf{r},t) + (1-\beta)\chi_g^p\sum_{g'=1}^{G}\nu\Sigma_{g'}^f(\mathbf{r},t)\varphi_{g'}(\mathbf{r},t) + \chi_g^d\sum_{j=1}^{J}\lambda_j C_j(\mathbf{r},t), \quad g=1,\ldots,G, \tag{1}$$

$$\frac{\partial C_j(\mathbf{r},t)}{\partial t} = \beta_j\sum_{g'=1}^{G}\nu\Sigma_{g'}^f(\mathbf{r},t)\varphi_g(\mathbf{r},t) - \lambda_j C_j(\mathbf{r},t), \quad j=1,\ldots,J, \tag{2}$$

where, in standard notation, g is the neutron energy group index; G is the total number of energy groups; j is the delayed neutron precursor group index; J is the total number of delayed precursor groups; φ_g is the neutron flux in energy group g; D_g is the diffusion coefficient in group g; Σ_g^r is the macroscopic removal cross section for group g; χ_g^p is the prompt neutron fission spectrum in group g; χ_g^d is the delayed neutron fission spectrum in group g; $\nu\Sigma_g^f$ is the macroscopic production cross section for group g; $\Sigma_{gg'}^s$ is the macroscopic scattering cross section from group g' to group g; β_j is the delayed neutron yield fraction, group j; β is the total yield of delayed neutrons per fission; λ_j is the delayed neutron decay constant, group j; C_j is the delayed neutron precursor group concentration.

The system of equations (1)-(2) are completed by suitable boundary and initial conditions. To obtain a numerical solution to this initial problem, equations (1)-(2) are discretized on an X-Y-Z or triangular-Z mesh system imposed on the reactor region by using the mesh-centered finite-difference method. The resulting system of ordinary differential equations can be written in the matrix form as

$$v_g^{-1}\frac{d\boldsymbol{\varphi}_g(t)}{dt} = -\mathbf{L}_g\boldsymbol{\varphi}_g(t) + \sum_{g'\neq g}\mathbf{T}_{gg'}\boldsymbol{\varphi}_{g'}(t) + (1-\beta)\chi_g^p\sum_{g'=1}^{G}\mathbf{F}_{g'}\boldsymbol{\varphi}_{g'}(t) + \chi_g^d\sum_{j=1}^{J}\lambda_j\mathbf{C}_j(t), \quad g=1,\ldots,G, \tag{3}$$

$$\frac{d\mathbf{C}_j(t)}{dt} = \beta_j\sum_{g'=1}^{G}\mathbf{F}_{g'}\boldsymbol{\varphi}_g(t) - \lambda_j\mathbf{C}_j(t), \quad j=1,\ldots,J, \tag{4}$$

where $\boldsymbol{\varphi}_g$ is the neutron flux vector, group g; $\mathbf{C}_j$ is the delayed neutron precursor vector, group j; $\mathbf{L}_g$ is the leakage plus removal matrix operator, group g; $\mathbf{T}_{gg'}$ is the diagonal scattering matrix, group g' to

group g; $\mathbf{F}_g$ is the diagonal production matrix, group g; $\boldsymbol{\chi}_g^p$ is the diagonal prompt neutron fission spectrum matrix, group g; $\boldsymbol{\chi}_g^d$ is the diagonal delayed neutron fission spectrum matrix, group g; $\mathbf{v}_g^{-1}$ is the diagonal inverse neutron velocity matrix, group g.

An application of the fully-implicit scheme to the neutron kinetics equations (3) in combination with the "time integrated" approximation to the delayed neutron precursors equations (4) (Stacey, 1969) results in the next equation set

$$\tilde{\mathbf{M}}\boldsymbol{\varphi}(t+\Delta t) = \tilde{\mathbf{F}}\boldsymbol{\varphi}(t+\Delta t) + \mathbf{q}, \tag{5}$$

$$\mathbf{C}_j(t+\Delta t) = \alpha_j \mathbf{C}_j(t) + \frac{1-\alpha_j}{\lambda_j}\beta_j \mathbf{F}\boldsymbol{\varphi}(t+\Delta t), \tag{6}$$

where $\alpha_m = \exp(-\lambda_m \Delta t)$; $\boldsymbol{\varphi} = \mathrm{col}\,\{\boldsymbol{\varphi}_1, \boldsymbol{\varphi}_2, \ldots, \boldsymbol{\varphi}_G\}$; $\mathbf{F} = \{\mathbf{F}_1, \mathbf{F}_2, \ldots, \mathbf{F}_G\}$ is the matrix of order Kx(K*G); $\mathbf{q} = \frac{1}{\Delta t}\mathbf{v}^{-1}\boldsymbol{\varphi}(t) + \boldsymbol{\chi}^d \sum_{j=1}^{J} \lambda_j \alpha_j \mathbf{C}_j(t)$; $\mathbf{v}^{-1} = \mathrm{col}\,\{\mathbf{v}_1^{-1}, \mathbf{v}_2^{-1}, \ldots, \mathbf{v}_G^{-1}\}$; $\boldsymbol{\chi}^d = \mathrm{col}\,\{\boldsymbol{\chi}_1^d, \boldsymbol{\chi}_2^d, \ldots, \boldsymbol{\chi}_G^d\}$ and $\tilde{\mathbf{M}}$, $\tilde{\mathbf{F}}$ are square matrices of order K*G.

The matrix $\tilde{\mathbf{M}}$ is given by

$$\tilde{\mathbf{M}} = \begin{bmatrix} \tilde{\mathbf{A}}_1 & & & & \\ \mathbf{T}_{21} & \tilde{\mathbf{A}}_2 & & \mathbf{0} & \\ \cdot & \cdot & \cdot & & \\ \cdot & & \cdot & \cdot & \\ \cdot & & & \cdot & \cdot \\ \mathbf{T}_{G1} & \mathbf{T}_{G2} & \cdot & \cdot & \cdot \; \mathbf{T}_{G,G-1} \; \tilde{\mathbf{A}}_G \end{bmatrix},$$

where $\mathbf{0}$ is a null matrix and $\tilde{\mathbf{A}}_g = \mathbf{L}_g + \mathbf{v}_g^{-1}\frac{1}{\Delta t}$.

The matrix $\tilde{\mathbf{F}}$ in Eq. (5) is defined by

$$\tilde{\mathbf{F}} = \left[\boldsymbol{\chi}^p(1-\beta) + \boldsymbol{\chi}^d \sum_{j=1}^{J} \beta_j (1-\alpha_j)\right]\mathbf{F},$$

where $\boldsymbol{\chi}^p = \mathrm{col}\,\{\boldsymbol{\chi}_1^p, \boldsymbol{\chi}_2^p, \ldots, \boldsymbol{\chi}_G^p\}$.

Thus, at each time step we should solve the neutron flux equations (5) with respect to the neutron flux vector $\boldsymbol{\varphi}(t+\Delta t)$ and then recalculate the delayed neutron precursors $\mathbf{C}_m(t+\Delta t)$ from Eq. (6). The neutron flux equations (5) can be rewritten in compact matrix form as

$$\boldsymbol{\varphi} = \mathbf{B}\boldsymbol{\varphi} + \mathbf{f}, \tag{7}$$

where $\mathbf{B} = \tilde{\mathbf{M}}^{-1}\tilde{\mathbf{F}}$, $\mathbf{f} = \tilde{\mathbf{M}}^{-1}\mathbf{q}$.

We assume in the context that follows that the space-time finite-difference approximations have been made in such a way that

1) matrix B is symmetric;

2) matrix B has K*G real eigenvalues that can be ordered as

$$m \equiv \lambda_{K*G} \le \ldots \le \lambda_i \le \lambda_{i-1} \ldots \le \lambda_2 < \lambda_1 \equiv M < 1; \text{ and}$$

3) corresponding eigenvectors $\{\boldsymbol{\psi}_i\}$ form a basis of the K*G-dimensional vector space.

III. BASIC ITERATION METHODS

The discretized neutron flux equations can be solved iteratively at each time step using the Fission Source Iteration (FSI) method that can be written as

$$\tilde{\mathbf{M}}\boldsymbol{\varphi}^{(n+1)} = \tilde{\mathbf{F}}\boldsymbol{\varphi}^{(n)} + \mathbf{q}, \text{ or } \boldsymbol{\varphi}^{(n+1)} = \mathbf{B}\boldsymbol{\varphi}^{(n)} + \mathbf{f}, \tag{8}$$

where n is the fission source (outer) iteration number. The error vector $\varepsilon^{(n)}$ of iteration process (8) is defined by

$$\varepsilon^{(n)} \equiv \varphi^{(n)} - \varphi,$$

where φ is a unique solution of the equation (7). The error vector $\varepsilon^{(n)}$ relates to the initial error vector $\varepsilon^{(0)}$ through the expression

$$\varepsilon^{(n)} = B\varepsilon^{(n-1)} = B^2\varepsilon^{(n-2)} = \ldots = B^n\varepsilon^{(0)}$$

and the convergence rate of the FSI method is defined by

$$R_{FSI}(B) = -\ln(S(B)),$$

where $S(B)$ is the spectral radius of the iteration matrix.

For many practical applications the spectral radius $S(B)$ is close to unity and the convergence rate of the FSI method is very slow. For example, let us consider a delayed critical transient calculation with relatively large time step sizes. Assuming that $\chi^d \approx \chi^p$ and neglecting the terms $\frac{1}{\Delta t}v_g^{-1}$ in the matrix $\tilde{M}$, we obtain

$$S(B) = S\left(\tilde{M}^{-1}\tilde{F}\right) \approx S\left(M^{-1}\chi^p(1-\sum_{j=1}^{J}\beta_j\alpha_j)F\right) = (1-\sum_{j=1}^{J}\beta_j\alpha_j)k_{eff},$$

where $k_{eff} = S\left(M^{-1}\chi^p F\right)$ is the multiplication factor of the steady-state problem.

Letting $k_{eff} \approx 1$ and using one group of delayed neutron precursors with $\lambda = 0.1$ s and b=0.0065 for the time step size Δt=0.25 s, we obtain $S(B) \approx 0.994$. Therefore there is a strong motivation for the use of an efficient acceleration technique for the fission source iteration method.

Let us consider one acceleration technique, the Modified Fission Source Iteration (MFSI) method (Zimin and Schukin, 1992). The residual vector $\delta^{(n)}$ of the FSI method is defined by

$$\delta^{(n)} \equiv B\varphi^{(n)} + f - \varphi^{(n)}.$$

The residual vector $\delta^{(n)}$ can be expressed through the initial residual vector $\delta^{(0)}$ as

$$\delta^{(n)} = B^n\delta^{(0)}.$$

Expanding the initial residual vector $\delta^{(0)}$ into eigenvectors $\{\psi_i\}$ as

$$\delta^{(0)} = \sum_{i=1}^{K*G} c_i\psi_i$$

after n iterations of the FSI method we obtain

$$\delta^{(n)} = (\lambda_1)^n\left\{c_1\psi_1 + \sum_{i=1}^{K*G}\left(\frac{\lambda_i}{\lambda_1}\right)^n c_i\psi_i\right\}.$$

Therefore, during outer iterations of the FSI method the residual vector $\delta^{(n)}$ converges to the eigenvector ψ_1 of the iteration matrix B. A convergence of the residual vectors $\delta^{(n)}$ to the eigenvector ψ_1 can be significantly faster then the convergence of the iterative approximations $\{\varphi^{(n)}\}$ to the exact solution. The error vector $\varepsilon^{(n)}$ of the FSI method is related to the residual vector $\delta^{(n)}$ by

$$\varepsilon^{(n)} = (B-I)^{-1}\delta^{(n)}.$$

Then, the exact solution of the neutron flux equations can be written in the form

$$\varphi = \varphi^{(n)} - \varepsilon^{(n)} = \varphi^{(n)} + (I-B)^{-1}\delta^{(n)}.$$

Therefore, if the residual vector $\delta^{(n)}$ contains only the eigenvector ψ_1 of the matrix B, the improved approximation $\varphi_{ext}^{(n)}$ to the solution φ can be obtained from

$$\varphi_{ext}^{(n)} \approx \varphi^{(n)} + \frac{1}{1-\lambda_1}\delta^{(n)}, \tag{9}$$

where the analytical summation of the Neumann expansion of the matrix $(I-B)^{-1}$ is used. The refinement of the iterative solution by (9) is called the Lyusternik acceleration technique (Marchuk and Lebedev, 1981) or Aitken extrapolation procedure (Fox, 1964).

The resulting iteration procedure of the neutron kinetics equations solution can be written in the form

$$\delta^{(0)} = B\varphi^{(0)} + f - \varphi^{(0)}, \tag{10}$$

$$\delta^{(n+1)} = B\delta^{(n)}, \qquad n \geq 0, \tag{11}$$

$$\varphi^{(n+1)} = \varphi^{(n)} + \delta^{(n)}, \qquad n \geq 0, \tag{12}$$

and the first eigenvalue estimate can be computed from the Rayleigh quotient

$$\lambda_1^{(n)} = \frac{\left(B\delta^{(n)}, \delta^{(n)}\right)}{\left(\delta^{(n)}, \delta^{(n)}\right)}. \tag{13}$$

When the convergence of the residual vector $\delta^{(n)}$ to the eigenvector ψ_1 is attained, the analytical refinement (9) is used.

The iteration procedure (10)-(13) with the analytical refinement (9) was called the Modified Fission Source Iteration (MFSI) method (Zimin and Schukin, 1992). The calculations of the delayed critical transients in a small-sized thermal reactor demonstrated that the number of iterations of the MFSI method may be an order of magnitude less than the number of iterations of the FSI method (Zimin and Schukin, 1992). However, for calculations of operational power reactors, especially with a fine spatial mesh, the convergence of the MFSI method is rather slow. The additional results of the neutron kinetics benchmark problems calculations using the MFSI method will be presented in Section VIII.

IV. CHEBYSHEV ACCELERATION PROCEDURE

We will consider an application of the Chebyshev acceleration procedure (Hageman and Young, 1981) to acceleration of the outer iterative process. Let us define the Chebyshev polynomial sequence $\{P_{n,E}(x)\}$ by

$$P_{n,E}(x) = \frac{T_n(w_E(x))}{T_n(w_E(1))},$$

where $T_n(x)$ is the Chebyshev polynomial of degree n, $w_E(x) = \dfrac{2x - M_E - m_E}{M_E - m_E}$; m_E and M_E are the estimates of certain eigenvalue bounds of the matrix B, that satisfy the conditions

$$m_E \leq m \quad \text{and} \quad m_E \leq M_E \leq M.$$

The Chebyshev polynomials $P_{n,E}(x)$ satisfy the recurrent expressions

$$P_o(x) = 1,$$

$$P_1(x) = \gamma x - \gamma + 1,$$

$$P_{n+1}(x) = \rho_{n+1}(\gamma x + 1 - \gamma)P_n(x) + (1 - \rho_{n+1})P_{n-1}(x), \qquad n \geq 1,$$

where $\gamma = 2/(2 - M_E - m_E)$, $\rho_1 = 1$, $\rho_2 = \left(1 - 0.5\sigma_E^2\right)^{-1}$, $\rho_{n+1} = \left(1 - 0.25\sigma_E^2\rho_n\right)^{-1}$, $n \geq 2$; and $\sigma_E = 1/w_E(1) = \dfrac{M_E - m_E}{2 - M_E - m_E}$.

The iterative approximations $\{\tilde{\varphi}^{(n)}\}$ of the Chebyshev acceleration procedure can be obtained from the following three-term recurrent expressions

$$\tilde{\varphi}^{(1)} = \gamma(B\tilde{\varphi}^{(0)} + f) + (1 - \gamma)\tilde{\varphi}^{(0)}, \tag{14}$$

$$\tilde{\varphi}^{(n+1)} = \rho_{n+1}\left(\gamma(B\tilde{\varphi}^{(n)} + f) + (1 - \gamma)\tilde{\varphi}^{(n)}\right) + \left(1 - \rho_{n+1}\right)\tilde{\varphi}^{(n-1)}, \qquad n \geq 1. \tag{15}$$

The error vector $\tilde{\varepsilon}^{(n)} \equiv \tilde{\varphi}^{(n)} - \varphi$ and the residual vector $\tilde{\delta}^{(n)} \equiv B\tilde{\varphi}^{(n)} + f - \tilde{\varphi}^{(n)}$ of the Chebyshev acceleration procedure satisfy the following relations

$$\tilde{\delta}^{(n)} = P_{n,E}(B)\tilde{\delta}^{(0)}, \qquad n \geq 0, \quad \text{and} \tag{16}$$

$$\tilde{\varepsilon}^{(n)} = (B - I)^{-1}\tilde{\delta}^{(n)}, \qquad n \geq 0, \tag{17}$$

where $P_{n,E}(B)$ is a matrix polynomial corresponding to the algebraic polynomial $P_{n,E}(x)$.

The norm of the error vector $\tilde{\varepsilon}^{(n)}$ satisfies the inequalities

$$\left\|\tilde{\varepsilon}^{(n)}\right\| \le \left\|\mathbf{P}_{n,E}(\mathbf{B})\right\| \left\|\tilde{\varepsilon}^{(0)}\right\| \le \bar{S}\left(\mathbf{P}_{n,E}(\mathbf{B})\right) \left\|\tilde{\varepsilon}^{(0)}\right\|,$$

where $\bar{S}\left(\mathbf{P}_{n,E}(\mathbf{B})\right) = \max\limits_{m \le x \le M} \left|P_{n,E}(x)\right|$ is a virtual spectral radius of the matrix polynomial $\mathbf{P}_{n,E}(\mathbf{B})$. If $m_E = m$ and $M_E = M$, we have the matrix polynomial $\mathbf{P}_{n,E}(\mathbf{B})$ with the minimal virtual spectral radius. The corresponding acceleration procedure, called the Chebyshev Semi-Iterative (CSI) method (Varga, 1962), has a minimal norm of the error vector and in this sense optimizes the convergence of outer iterations of the FSI method. The convergence rate of the Chebyshev semi-iterative method is determined by the virtual spectral radius $\bar{S}\left(\mathbf{P}_{n,E}(\mathbf{B})\right)$, that, in this case, can be written as

$$\bar{S}\left(\mathbf{P}_{n,E}(\mathbf{B})\right) = 1/T_n\left(\frac{2-M-m}{M-m}\right).$$

Let us consider behavior of the residual vector $\tilde{\delta}^{(n)}$ during the Chebyshev iterations. Expanding the initial residual vector $\tilde{\delta}^{(0)}$ into eigenvectors $\{\psi_i\}$ as

$$\tilde{\delta}^{(0)} = \sum_{i=1}^{K*G} c_i \psi_i$$

and using (16) we can write the residual vector $\tilde{\delta}^{(n)}$ in the form

$$\tilde{\delta}^{(n)} = P_{n,E}(\lambda_1)\left\{c_1\psi_1 + \sum_{i=1}^{K*G} \frac{P_{n,E}(\lambda_i)}{P_{n,E}(\lambda_1)} c_i \psi_i\right\}. \tag{18}$$

It has been shown (Hageman and Young, 1981) that if the parameters m_E and M_E satisfy the next conditions

$$m_E \le m \quad \text{and} \quad m_E \le M_E < M \tag{19}$$

the residual vectors $\tilde{\delta}^{(n)}$ converge to the eigenvector ψ_1 of the iteration matrix $\mathbf{B}$, and the convergence rate is optimal when

$$m_E = m \quad \text{and} \quad M_E = \lambda_2. \tag{20}$$

The convergence of the residual vectors to the eigenvector ψ_1 of the iteration matrix $\mathbf{B}$ is called the *secondary iterative process* (Hageman and Young, 1981) in contrast to the *main iterative process*, where the iterative approximations converge to the exact solution. If the first eigenvalue of the iteration matrix $\mathbf{B}$ is close to unity, the convergence of the optimized secondary iterative process with eigenvalue estimates (20) may be significantly faster then the convergence of the Chebyshev semi-iterative method, that optimizes the convergence rate of the main iterative process.

The error vector $\tilde{\varepsilon}^{(n)}$ and the residual vector $\tilde{\delta}^{(n)}$ are related by (17). Therefore, when the convergence of the residual vector to the eigenvector ψ_1 is attained, we can again use the Neumann expansion of the matrix $(\mathbf{I}-\mathbf{B})^{-1}$ and obtain the improved approximation $\tilde{\varphi}_{ext}^{(n)}$ to the solution φ from

$$\tilde{\varphi}_{ext}^{(n)} = \tilde{\varphi}^{(n)} + \frac{1}{1-\lambda_1}\tilde{\delta}^{(n)} \tag{21}$$

The application of the analytical refinement (21) requires an accurate estimate of the eigenvalue λ_1 during the Chebyshev iterations. The Chebyshev acceleration procedure (14)-(15) can be rewritten in the form

$$\tilde{\delta}^{(0)} = \mathbf{B}\tilde{\varphi}^{(0)} + \mathbf{f} - \tilde{\varphi}^{(0)}, \tag{22}$$

$$\theta^{(n)} = \mathbf{B}\tilde{\delta}^{(n)}, \quad n \ge 0, \tag{23}$$

$$\tilde{\varphi}^{(n+1)} = \rho_{n+1}(\gamma\tilde{\delta}^{(n)} + \tilde{\varphi}^{(n)}) + (1-\rho_{n+1})\tilde{\varphi}^{(n-1)}, \quad n \ge 0, \tag{24}$$

$$\tilde{\delta}^{(n+1)} = \rho_{n+1}(\gamma\theta + (1-\gamma)\tilde{\delta}^{(n)}) + (1-\rho_{n+1})\tilde{\delta}^{(n-1)}, \quad n \ge 0, \tag{25}$$

and the eigenvalue estimate $\lambda_1^{(n)}$ can be obtained from

$$\lambda_1^{(n)} = \frac{\left(\mathbf{B}\tilde{\delta}^{(n)}, \tilde{\delta}^{(n)}\right)}{\left(\tilde{\delta}^{(n)}, \tilde{\delta}^{(n)}\right)}. \tag{26}$$

The proposed combination of the Çhebyshev acceleration procedure (22)-(26) with the optimum eigenvalues estimates (20) and the analytical refinement of the obtained approximation (21) is called here the *Chebyshev Semi-Analytical (CSA) method.*

During the iteration procedure (22)-(26), we can estimate the error that will appear as a result of the application of the analytical refinement (21) in the following manner. Defining the error vector $\tilde{\varepsilon}_{ext}^{(n)}$ by

$$\tilde{\varepsilon}_{ext}^{(n)} = \tilde{\varphi}_{ext}^{(n)} - \varphi .$$

and using the expansion (18), we have

$$\tilde{\varepsilon}_{ext}^{(n)} = \tilde{\varphi}^{(n)} + \frac{\tilde{\delta}^{(n)}}{1-\lambda_1} - \varphi = \frac{\tilde{\delta}^{(n)}}{1-\lambda_1} - (\mathbf{I}-\mathbf{B})^{-1}\tilde{\delta}^{(n)} =$$

$$\sum_{i=1}^{K*G}\left[\frac{1}{1-\lambda_1} - \frac{1}{1-\lambda_i}\right] P_{n,E}(\lambda_i)\, c_i \psi_i = \sum_{i=1}^{K*G}\left[\frac{\lambda_1-\lambda_i}{(1-\lambda_i)(1-\lambda_1)}\right] P_{n,E}(\lambda_i)\, c_i \psi_i .$$

Taking into account that

$$\tilde{\delta}^{(n)} = \sum_{i=1}^{K*G} P_{n,E}(\lambda_i)\, c_i \psi_i , \quad \mathbf{B}\tilde{\delta}^{(n)} = \sum_{i=1}^{K*G} P_{n,E}(\lambda_i)\, \lambda_i c_i \psi_i \quad \text{and} \quad |1-\lambda_i| \geq |1-\lambda_2| \text{ for all } i \geq 2 ,$$

we can obtain the estimate of the norm of the error vector $\tilde{\varepsilon}_{ext}^{(n)}$ from

$$\left\|\tilde{\varepsilon}_{ext}^{(n)}\right\| \leq \frac{1}{(1-\lambda_1)(1-\lambda_2)}\left\|\lambda_1\tilde{\delta}^{(n)} - \mathbf{B}\tilde{\delta}^{(n)}\right\| . \tag{27}$$

Using (27) and the approximation $\varphi \approx \tilde{\varphi}^{(n+1)}$ a relative norm of the error vector can be estimated from

$$E \leq \frac{1}{(1-\lambda_1)(1-\lambda_2)} \frac{\left\|\lambda_1^{(n)}\tilde{\delta}^{(n)} - \mathbf{B}\tilde{\delta}^{(n)}\right\|_2}{\left\|\tilde{\varphi}^{(n+1)}\right\|_2} .$$

Thus, the Chebyshev iterations (22)-(26) are performed until the evaluated relative norm of the error vector is less than a given tolerance and then the analytical refinement (21) is applied.

V. ESTIMATION OF THE OPTIMUM ITERATION PARAMETERS

In order to optimize convergence rate of the Chebyshev semi-analytical method it is essential to estimate the second eigenvalue λ_2 of the iteration matrix **B**. Actually, we also have to know a lower bound of the eigenvalues. However we can assume that all eigenvalues of the matrix **B** are nonnegative and the estimate of the smallest eigenvalue $m_E = 0$ can be used. The initial estimate of the second eigenvalue λ_2 can be obtained in advance of the transient calculation from the results of the first time step calculation using the MFSI method. We note that the Chebyshev iteration procedure (22)-(26) reduces to the MFSI method if $\rho_n = 1$ for all $n \geq 0$ and $\gamma = 1$.

Let us define the residual vector of the secondary iteration process $\Delta^{(n)}$ by

$$\Delta^{(n)} \equiv \lambda_1^{(n)}\delta^{(n)} - \mathbf{B}\delta^{(n)} ,$$

and the corresponding residual vector quotient $Q^{(n+1)}$ by

$$Q^{(n+1)} \equiv \left\|\Delta^{(n+1)}\right\| / \left\|\Delta^{(n)}\right\| . \tag{28}$$

Using the MFSI method we have

$$\lim_{n\to\infty} Q^{(n+1)} = \lambda_2$$

and therefore the initial estimate of the second eigenvalue can be obtained from Eq. (28) after a limited number of outer iterations.

The obtained estimate is used as the initial approximation in computing the Chebyshev iteration parameters for the transient calculation. The eigenvalues of the matrix **B** may change during the calculated transient. It is therefore desirable to use an adaptive procedure for improvement of the λ_2 estimate. The adaptive Chebyshev procedure (Hageman and Young, 1981), proposed for the

estimation of the spectral radius of the iteration matrix **B**, can be easily modified for the estimation of the second eigenvalue λ_2. The procedure is based on a comparison of the observed convergence rate of the Chebyshev iterations with the theoretical convergence rate of the Chebyshev acceleration procedure where the optimum iteration parameters are employed. The theoretical background and computational strategy of the adaptive Chebyshev procedure are given in (Hageman and Young, 1981). Here we will discuss only the modifications of the procedure for our purposes.

Let us consider the Chebyshev iteration procedure (22)-(26), where the polynomial sequence $\{P_{n,E}(x)\}$ is given here by

$$P_{n,E}(x) = \frac{T_n(w_E(x))}{T_n(w_E(1))},$$

where $w_E(x) = \dfrac{2x - \lambda_2^E - m_E}{\lambda_2^E - m_E}$, and the eigenvalue estimates λ_2^E and m_E satisfy the next conditions

$$m_E \le \lambda_2^E < \lambda_2 \quad \text{and} \quad m_E \le m. \tag{29}$$

Assuming $\lambda_1^{(n)} \approx \lambda_1$ for all $n \ge 0$, and using the expansion (18), the residual vector $\Delta^{(n)}$ can be approximated by

$$\Delta^{(n)} \approx P_{n,E}(\lambda_1)\left\{\sum_{i=2}^{K\cdot G} \frac{P_{n,E}(\lambda_i)}{P_{n,E}(\lambda_1)}(\lambda_1 - \lambda_i)c_i\ \Psi_i\right\}.$$

Then the norm of the residual vector $\Delta^{(n)}$ satisfies the following inequalities

$$\left\|\Delta^{(n)}\right\| \le P_{n,E}(\lambda_1) \max_{K\cdot G \le i \le 2}\left\{\frac{P_{n,E}(\lambda_i)}{P_{n,E}(\lambda_1)}\right\}\left\|\Delta^{(0)}\right\|$$

and

$$\left\|\Delta^{(n)}\right\| \le P_{n,E}(\lambda_1)\,\alpha(n)\left\|\Delta^{(0)}\right\|, \tag{30}$$

where $\alpha(n)$ is the convergence factor (Hageman and Young, 1981) defined by

$$\alpha(n) = \max_{m \le x \le \lambda_2} \left|P_{n,E}(x)/P_{n,E}(\lambda_1)\right|.$$

If the eigenvalue estimates λ_2^E and m_E satisfy the conditions (29), the convergence factors $\alpha(n)$ satisfy the following inequalities

$$\alpha(n) \le \frac{T_n(w_E(\lambda_2))}{T_n(w_E(\lambda_1))}, \text{ if } \lambda_2^E \le \lambda_2;$$

or

$$\alpha(n) \le \frac{1}{T_n(w_E(\lambda_1))}, \text{ if } \lambda_2^E > \lambda_2. \tag{31}$$

If the estimate λ_2^E of the second eigenvalue satisfies the condition $\lambda_2^E \ge \lambda_2$, then from (30) and (31) we obtain that

$$\left\|\Delta^{(n)}\right\| / \left\|\Delta^{(0)}\right\| \le P_{n,E}(\lambda_1)\frac{1}{T_n(w_E(\lambda_1))} = \frac{1}{T_n(w_E(1))} \tag{32}$$

Therefore, if condition (32) is not satisfied, i.e.

$$\left\|\Delta^{(n)}\right\| / \left\|\Delta^{(0)}\right\| > \frac{1}{T_n(w_E(1))} \tag{33}$$

we have the strict confirmation that $\lambda_2^E < \lambda_2$.

For practical applications, in order to eliminate the generation of the new Chebyshev polynomial at each outer iteration, a damping factor F was introduced (Hageman and Young, 1981), and the condition (33) is replaced by the following

$$\left\|\Delta^{(n)}\right\| / \left\|\Delta^{(0)}\right\| > \left(\frac{1}{T_n(w_E(1))}\right)^F = \left(\frac{2r^{n/2}}{1+r^n}\right)^F, \tag{34}$$

where $r = \left(1-\sqrt{1-\sigma_E^2}\right)/\left(1+\sqrt{1-\sigma_E^2}\right)$ and $\sigma_E = \dfrac{M_E - m_E}{2 - M_E - m_E}$.

As a result we obtain the average convergence rate that may be F times slower than the optimal convergence rate of the Chebyshev acceleration procedure. The acceptable values of the damping factor F would lie in the interval [0.65,0.8].

If the condition (34) is satisfied, we could obtain an improved estimate $\lambda_2^E(new)$ as the maximum real solution of the Chebyshev equation

$$T_n(w_E(x))/T_n(w_E(1)) = \left\|\Delta^{(n)}\right\| / \left\|\Delta^{(0)}\right\|.$$

Letting

$$X = \left\|\Delta^{(n)}\right\| / \left\|\Delta^{(0)}\right\| \quad \text{and} \quad Z = \frac{2r^{n/2}}{(1+r^n)}$$

the solution of Chebyshev equation can be computed from

$$\lambda_2^E(new) = \frac{1}{2}\left[\lambda_2^E + m_E + \left(\frac{2-\lambda_2^E - m_E}{1+r}\right)\left(\frac{Y^2+r}{Y^2}\right)\right],$$

where $Y = \left[0.5\left(1+r^n\right)\left(X+\sqrt{X^2-Z^2}\right)\right]^{1/n}$.

The new estimate $\lambda_2^E(new)$ also satisfies the condition $\lambda_2^E(new) \le \lambda_2$ and the adaptive estimation procedure can be repeated for the new Chebyshev polynomial sequence.

VI. "OPTIMAL" INITIAL APPROXIMATION

During transient calculations for the CSI method we can take the solution obtained at the previous time step as the initial approximation for the next time step. The situation is quiet different for the CSA and MFSI methods because our purpose is not to obtain the initial iterative approximation which is close to the solution, but the initial residual vector which is close to the eigenvector of the iteration matrix. In order to satisfy this requirement we can take as an initial approximation for the new time step the neutron flux $\tilde{\varphi}^{(n+1)}(t)$ obtained at the last iteration of the previous time step calculation. As a result we obtain the residual vector $\tilde{\delta}^{(0)}$ which is a "good" approximation to the eigenvector ψ_1 of the iteration matrix **B**. In fact, letting

$$\mathbf{B}(t+\Delta t) = \mathbf{B}(t) + \delta\mathbf{B}, \quad \mathbf{f}(t+\Delta t) = \mathbf{f}(t) + \delta\mathbf{f}$$

and taking into account that

$$\tilde{\varphi}_{opt}^{(0)}(t+\Delta t) = \tilde{\varphi}^{(n+1)}(t) = \varphi(t) + \tilde{\varepsilon}^{(n+1)} = \varphi(t) + (\mathbf{B}-\mathbf{I})^{-1}\tilde{\delta}^{(n+1)}$$

we have

$$\tilde{\delta}^{(0)}(t+\Delta t) = \mathbf{B}(t+\Delta t)\tilde{\varphi}^{(n+1)} + \mathbf{f}(t+\Delta t) - \tilde{\varphi}^{(n+1)} = \tilde{\delta}^{(n+1)}(t) + \delta\mathbf{B}\tilde{\varphi}^{(n+1)} + \delta\mathbf{f}$$

Then, when $\delta\mathbf{B} \approx \mathbf{0}$ and $\delta\mathbf{f} \approx \mathbf{0}$, the residual vector $\tilde{\delta}^{(0)}$ is close to the eigenvector of the iteration matrix **B** and after a few iterations we can use the Aitken extrapolation procedure (21) in order to calculate the solution $\varphi(t+\Delta t)$.

Using the initial approximation from the previous time step we decrease the norm of the residual vector at each time step and after several time steps we obtain the initial residual vector which contains only $\delta\mathbf{B}\tilde{\varphi}^{(n+1)} + \delta\mathbf{f}$. This results in the increase of outer iteration numbers and the decrease of convergence stability. In order to eliminate these cases we introduce the parameter *alfa_res* that normalizes the initial residual vector at each time step. The initial neutron flux vector is replaced on

$$\tilde{\varphi}_{opt}^{(0)}(t+\Delta t) = \varphi(t) + alfa\_res\,(\mathbf{B}-\mathbf{I})^{-1}\tilde{\delta}^{(n+1)}, \tag{35}$$

where parameter *alfa_res* is computed from

$$alfa\_res = \frac{\left\| \tilde{\delta}^{(n+1)}(0+\Delta t) \right\|_2}{\left\| \tilde{\delta}^{(n+1)}(t) \right\|_2} \frac{\left\| \tilde{\varphi}(t) \right\|_2}{\left\| \tilde{\varphi}(0+\Delta t) \right\|_2}.$$

As a result the initial residual vector can be written as

$$\tilde{\delta}^{(0)}(t+\Delta t) = alfa\_res\ \tilde{\delta}^{(n+1)}(t) + \delta \mathbf{B} \tilde{\varphi}^{(n+1)} + \delta \mathbf{f}.$$

Numerical results of the Langenbuch-Maurer-Werner benchmark problem calculations given in Sect. VIII demonstrate that the "optimal" initial approximation (35) significantly decreases the number of outer iterations of the CSA and MFSI methods during transient calculations.

VII. INNER ITERATIVE PROCESS

In the previous sections we have assumed that at each outer iteration the exact solution of the group neutron flux equations is obtained. However, it is not the case in most multi-dimensional practical problems and the group neutron flux equations are usually solved approximately by using an iteration method. The iterative solution method of the group equations is called an inner iteration method and the corresponding iterations are called inner iterations. Computational efficiency of the resulting iteration procedure depends significantly on the consistency of the outer and inner iteration methods and we will discuss this problem in this section. The problem has been considered by several authors for steady-state eigenvalue calculations (Wachspress, 1966; Ferguson and Derstine, 1977; Hageman and Young, 1981). We will use the same approach for the analysis of the iteration procedures of the neutron kinetics equations solution.

At first let us consider the influence of inner iterations on the properties of the outer iteration matrix **B** of the basic FSI method. At each outer iteration n we must solve the group neutron flux equations (8) that can be rewritten in the form

$$\tilde{\mathbf{A}}_g \varphi_g^{(n)} = \mathbf{b}_g, \quad g=1,2,\ldots,G, \tag{36}$$

where $\mathbf{b}_g = \sum_{g'<g} \mathbf{T}_{g,g'} \varphi_{g'}^{(n)} + \left[\chi_g^p (1-\beta) + \chi_g^d \sum_{j=1}^{J} \beta_j (1-\alpha_j) \right] \mathbf{F} \varphi^{(n-1)}$.

We have G systems of the linear equations that can be solved using an iteration method. As the matrix $\tilde{\mathbf{A}}_g$ is symmetric and positive definite, any iterative methods, e.g., SOR, conjugate gradient or Chebyshev semi-iterative method, can be used to solve the equations (36). Let's consider an iterative procedure with a fixed number of inner iterations of the solution of the group equation (36). We define the iteration approximations obtained at the outer iteration n as a result of m_g inner iterations as $\varphi_g^{(m_g)}(n)$. If $\varphi_g(n)$ is the exact solution of the group equations (36) at the outer iteration n, the error vector $\varepsilon_g^{(m_g)}(n)$ of the inner iteration process

$$\varepsilon_g^{(m_g)}(n) = \varphi_g^{(m_g)}(n) - \varphi_g(n),$$

relates to the initial error vector $\varepsilon_g^{(0)}(n)$ through the expression

$$\varepsilon_g^{(m_g)}(n) = \mathbf{Q}_g^{(m_g)} \varepsilon_g^{(0)}(n), \tag{37}$$

where $\mathbf{Q}_g^{(m_g)}$ is the convergent iteration error matrix (Hageman and Young, 1981) determined by the inner iteration method.

If the inner iterative process starts with the initial approximation from the previous outer iteration, i.e. $\varphi_g^{(0)}(n) = \varphi_g^{(m_g)}(n-1)$, from (36), (37) we have

$$\varphi_g^{(m_g)}(n) = \mathbf{Q}_g^{(m_g)} \varphi_g(n-1) + (\mathbf{I} - \mathbf{Q}_g^{(m_g)}) \tilde{\mathbf{A}}_g^{-1} \mathbf{b}_g. \tag{38}$$

Defining

$$\mathbf{Q}^{(m)} = \mathrm{diag}\{\mathbf{Q}_1^{(m_1)}, \mathbf{Q}_2^{(m_1)}, \ldots, \mathbf{Q}_G^{(m_G)}\} \text{ and } \varphi^{(m)}(n) = \mathrm{col}\{\varphi_1^{(m_1)}(n), \varphi_2^{(m_2)}(n), \ldots, \varphi_G^{(m_G)}(n)\},$$

we can rewrite the equations (38) in the compact matrix form

$$\boldsymbol{\varphi}^{(m)}(n) = \left(\tilde{\mathbf{M}}^{-1}\tilde{\mathbf{F}}\left[\mathbf{I} - \mathbf{Q}^{(m)}\right] + \mathbf{Q}^{(m)}\right)\boldsymbol{\varphi}^{(m)}(n-1) + (\mathbf{I} - \mathbf{Q}^{(m)})\tilde{\mathbf{M}}^{-1}\mathbf{q}$$

or

$$\boldsymbol{\varphi}^{(m)}(n) = \tilde{\mathbf{B}}\boldsymbol{\varphi}^{(m)}(n-1) + \tilde{\mathbf{f}}, \tag{39}$$

where $\tilde{\mathbf{B}} = \mathbf{B}\left[\mathbf{I} - \mathbf{Q}^{(m)}\right] + \mathbf{Q}^{(m)}$, and $\tilde{\mathbf{f}} = (\mathbf{I} - \mathbf{Q}^{(m)})\,\mathbf{f}$.

Then, if we solve the group neutron flux equations (36) using the inner iteration method, the outer Chebyshev acceleration procedure should be considered with respect to the basic iteration method defined by Eq. (39) instead of the one defined by Eq. (8). It is noted that, if the number of inner iterations $m_g \to \infty$ for all g=1, 2, . . . , G; then $\mathbf{Q}^{(m)} \to \mathbf{0}$, $\tilde{\mathbf{B}} \to \mathbf{B}$, $\tilde{\mathbf{f}} \to \mathbf{f}$ and the equations (38) and (8) are equivalent. The efficiency of the Chebyshev outer iterations depends significantly on the properties of the iteration matrix $\tilde{\mathbf{B}}$. Comparing the iteration matrices of the iteration procedures (39) and (8), we can conclude that the application of the inner iteration method changes the properties of the matrix **B** in two ways. *First*, the spectral radius and the second eigenvalue of the iteration matrix $\tilde{\mathbf{B}}$ are larger than the corresponding eigenvalues of the matrix **B**. This effect of the increase in the number of outer iterations is compensated by the decrease in the number of inner iterations and the total number of inner iterations usually decreases if a fewer number of inner iterations per outer iteration is specified. *Second*, the application of such iteration methods as SOR, Chebyshev semi-iterative and conjugate gradient methods, results in a convergent matrix $\mathbf{Q}^{(m)}$ that has negative and complex eigenvalues. The outer iteration matrix $\tilde{\mathbf{B}}$ will also have negative and complex eigenvalues, which can drastically affect the convergence of the outer Chebyshev acceleration procedure. However, this effect can be eliminated by the proper selection of the inner iteration method. For example, the iteration matrices of the point, line or block SSOR methods have only real nonnegative eigenvalues and therefore the iteration matrix $\tilde{\mathbf{B}}$ as well as the matrix **B** will also have real and nonnegative eigenvalues. As the matrix $\tilde{\mathbf{A}}_g$ is a positive definite *L*-matrix (Young, 1977), the SSOR method even with the relaxation factor being equal to unity should be quite efficient for this problem (Young, 1977). Therefore we use the symmetric Gauss-Seidel method (the SSOR method with the relaxation factor being equal to 1) for the solution of the group neutron flux equations. The matrix $\tilde{\mathbf{A}}_g$ is split into the form

$$\tilde{\mathbf{A}}_g = \mathbf{D}_g - \mathbf{C}_g^L - \mathbf{C}_g^U,$$

where $\mathbf{D}_g = \text{diag}\,\tilde{\mathbf{A}}_g$, $\mathbf{C}_g^L$ is a strictly lower triangular matrix with the same elements below the diagonal as $\tilde{\mathbf{A}}_g$, and $\mathbf{C}_g^U$ is a strictly upper triangular matrix with the same elements above the diagonal as $\tilde{\mathbf{A}}_g$. The symmetric Gauss-Seidel method is given by the formulas

$$\boldsymbol{\varphi}_g^{(m_g+1)}(n) = \mathbf{Q}_g\,\boldsymbol{\varphi}_g^{(m_g)}(n) + \mathbf{k}_g$$

where $\mathbf{Q}_g = (\mathbf{I} - \mathbf{D}_g^{-1}\mathbf{C}_g^L)^{-1}\,\mathbf{D}_g^{-1}\mathbf{C}_g^U\,(\mathbf{I} - \mathbf{D}_g^{-1}\mathbf{C}_g^U)^{-1}\mathbf{D}_g^{-1}\mathbf{C}_g^L$, $\mathbf{k} = (\mathbf{I} - \mathbf{D}_g^{-1}\mathbf{C}_g^U)^{-1}\,(\mathbf{I} - \mathbf{D}_g^{-1}\mathbf{C}_g^L)^{-1}\mathbf{b}_g$.

The convergent iteration error matrix $\mathbf{Q}_g^{(m_g)}$ of the Eq. (39) for the symmetric Gauss-Seidel method is defined by

$$\mathbf{Q}_g^{(m_g)} = \left(\mathbf{Q}_g\right)^{m_g}.$$

The last problem that we have addressed here in order to conclude our discussion of the inner iterations is reduced to the determination of the optimal number of inner iterations per outer iteration. We usually perform a few number of inner iterations per outer iteration for practical calculations. Executed calculations have shown that a smaller number of inner iterations per outer iteration minimizes the total number of inner iterations and computational time.

VIII. NUMERICAL RESULTS

The Chebyshev acceleration procedure described by (22)-(26) with analytical refinement (21) has been incorporated into a 3D computer code SKETCH (Schukin et.al., 1994). The implementation

of outer iteration methods in SKETCH code is illustrated in Table 1. The iteration procedure (21)-(25) allows us to realize various outer iterations methods depending on the values of the iteration parameters. If $m_E = m$ and $M_E = \lambda_2$, we get the outer iterations of the Chebyshev semi-analytical method (CSA); if $m_E = m$ and $M_E = \lambda_1$, we obtain the Chebyshev semi-iterative method (CSI); and if $\rho_n = 1$ for all $n \geq 0$ and $\gamma = 1$, the iteration procedure (22)-(26) reduces to the outer iterations of the MFSI method. The iterations of the CSA and MFSI methods were started with $\tilde{\varphi}^{(0)}(0+\Delta t) = 0$ for the first time step of calculations and the "optimal" initial approximation $\tilde{\varphi}^{(0)}_{opt}(t+\Delta t)$ (see Eq. (35)) for all other time steps. For the CSI method the initial vector $\tilde{\varphi}^{(0)}(t+\Delta t) = \varphi(t)$ minimizing the norm of the initial error vector was used. We usually perform several iterations of the FSI method before Chebyshev iterations in order to eliminate the eigenvectors corresponding to small eigenvalues from the initial residual vector. This approach improves the convergence of both the CSI and CSA methods. The eigenvalues λ_1^E and λ_2^E for the CSI and CSA methods were evaluated using the adaptive Chebyshev procedure, λ_2^E for the MFSI method was calculated using expression (27), and $\lambda_1^{(n)}$ for the MFSI and CSA methods was computed from (25). The symmetric Gauss-Seidel method was used for the solution of the group neutron flux equations at each outer iteration. All performed calculations were done with a fixed number of inner iterations per outer iteration (2 for the fast neutron flux equations and 1 for thermal neutron flux equations).

Table 1. Implementation of the outer iteration methods in the SKETCH code.

	Chebyshev Semi-Iterative Method	Modified Fission Source Iteration Method	Chebyshev Semi-Analytical Method
Initial Approximation	$\tilde{\varphi}^{(0)}(t+\Delta t) = \varphi(t)$	$\tilde{\varphi}^{(0)}(0+\Delta t) = 0$ & $\tilde{\varphi}^{(0)}_{opt}(t+\Delta t) = \varphi(t) + alfa\_res\,(\mathbf{B}-\mathbf{I})^{-1}\tilde{\delta}^{(n+1)}$	
Iterations	Chebyshev Iterations $M_E \leq \lambda_1$	Fission Source Iterations $\rho_n = 1,\ \gamma = 1$	Chebyshev iterations $M_E \leq \lambda_2$
Convergence Criterion	$\frac{1}{(1-\lambda_1^E)} \frac{\left\|\tilde{\delta}^{(n)}\right\|_2}{\left\|\tilde{\varphi}^{(n+1)}\right\|_2} \leq \zeta$	$\frac{1}{(1-\lambda_1^E)(1-\lambda_2^E)} \frac{\left\|\lambda_1^E\tilde{\delta}^{(n)} - \mathbf{B}\tilde{\delta}^{(n)}\right\|_2}{\left\|\tilde{\varphi}^{(n+1)}\right\|_2} \leq \zeta$	
Solution	$\varphi(t+\Delta t) = \tilde{\varphi}^{(n+1)}$	$\varphi(t+\Delta t) = \tilde{\varphi}^{(n+1)} + \frac{1}{1-\lambda_1^{(n)}}\tilde{\delta}^{(n+1)}$	

The comparison of these iteration methods was performed for two neutron kinetics benchmark problems: the homogeneous cube benchmark problems: (Ferguson and Hansen, 1973) and the Langenbuch-Maurer-Werner (LMW) benchmark problem (Langenbuch et. al., 1977).

The first problem is a delayed critical transient in a bare homogeneous cube, 200 cm on a side, with two neutron groups and one precursor group (Ferguson and Hansen, 1973). The perturbation consists of a uniform step decrease in the thermal group absorption cross section and has a reactivity worth of about 50 cents. The exact solution of the semi-discretized problem, discretized in space with mesh size 20 cm, had been obtained by using an eigenvector expansion technique (see Ref. 14 in Fergusson and Hansen, 1973). The thermal neutron flux at the reactor center during the transient is shown in Fig. 1. The problem was calculated by computer code SKETCH using the MFSI, CSI and CSA methods with mesh size 20 cm and different time step sizes. The tolerance ζ was equal to 10^{-5} for time step size 0.001 s; 5×10^{-5} for time step sizes 0.005 and 0.01 s; and 10^{-4} for all other calculations. The temporal truncation error of the fully-implicit scheme is shown in Fig. 2, where the

thermal neutron flux error is plotted as a function of time step size at 0.4 s into the transient. The iteration matrix $\tilde{\mathbf{B}}$ does not change during the transient, so the optimum iteration parameters for the Chebyshev semi-iterative method and the Chebyshev semi-analytical method can be estimated in advance from the result of the first time step calculations using the MFSI method. The comparisons of the convergence behavior of the CSI, CSA and MFSI method are presented in Fig. 3 (a)-(c) for the first time step of the transient calculations with time step sizes 0.001, 0.01 and 0.1 s, respectively. The average number of outer iterations of the CSA, CSI and MFSI methods is compared in Fig. 4 for different time step sizes. Presented results show that the convergence rate of the CSA method is always higher than that of the traditional CSI method and the CSA method is 2-5 times faster than the CSI method. The following benchmark has been calculated in order to compare the iterative methods on more realistic delayed critical transient problem.

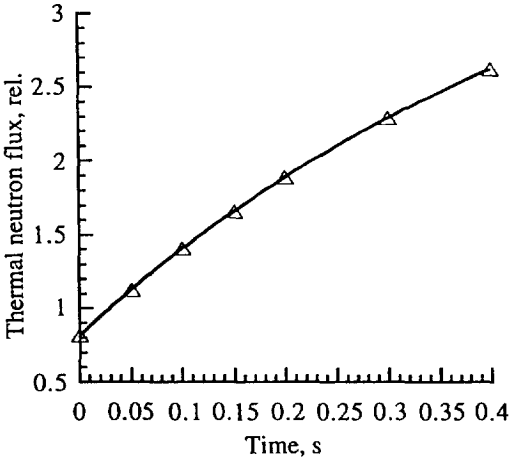

Fig. 1 Neutron flux at the reactor center versus time for the homogeneous cube benchmark problem.

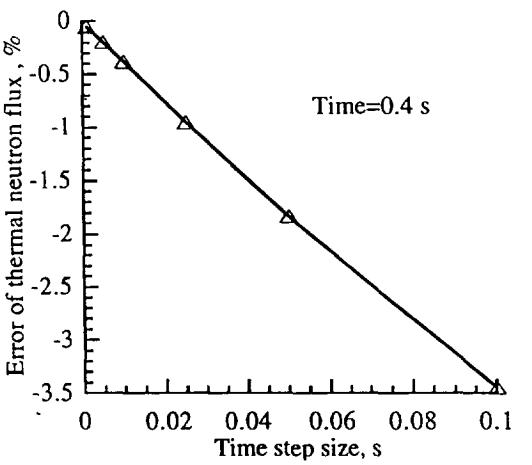

Fig. 2 Time discretization error of fully-implicit scheme for the homogeneous cube benchmark problem.

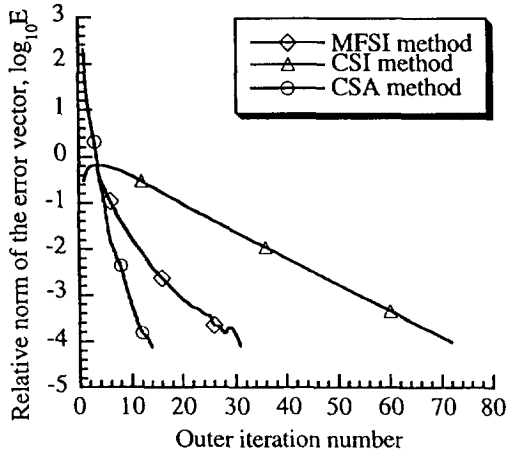

Fig. 3 (a) Convergence behavior of the MFSI, CSI and CSA methods for the homogeneous cube benchmark problem (first time step), Δt=0.1 s.

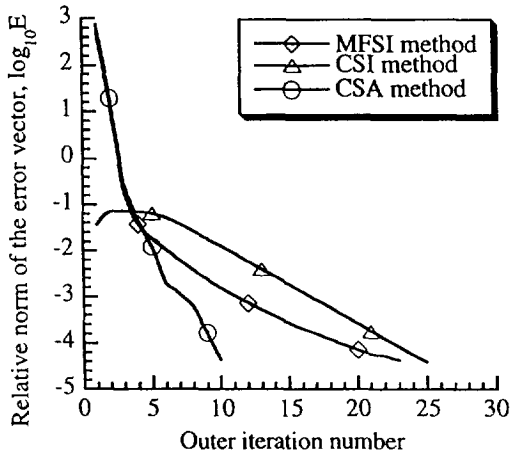

Fig. 3 (b) Convergence behavior of the MFSI, CSI and CSA methods for the homogeneous cube benchmark problem (first time step), Δt=0.01 s.

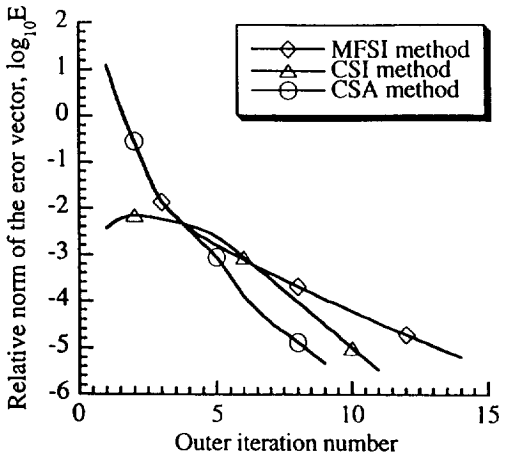

Fig. 3 (c) Convergence behavior of the MFSI, CSI and CSA methods for the homogeneous cube benchmark problem (first time step), Δt=0.001 s.

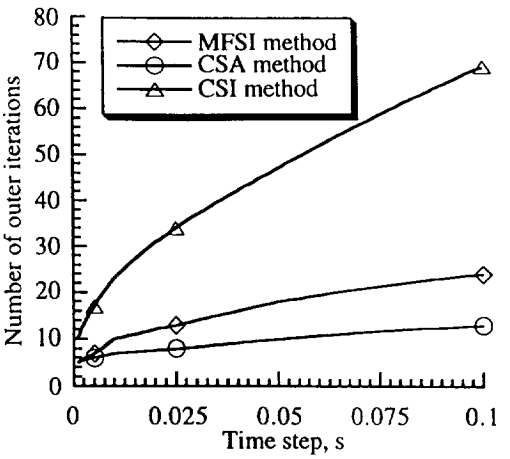

Fig. 4 Average number of outer iterations per time step as a function of time size for the homogeneous cube benchmark problem.

The second problem is an operational transient in a LWR model (Langenbuch et. al., 1977). The small-sized two-zone core consists of 77 assemblies, surrounded radially and axially by a water reflector. The transient is initiated by withdrawing a bank of four partially inserted control rods at the rate of 3 cm/s over the time interval from 0 to 26.7 s. The second bank of control rods is inserted at the same rate over the time from 7.5 to 47.5 s. The transient is followed for 60 s. The numerical solution of this problem had been obtained using several nodal computer codes (Langenbuch et. al., 1977; Smith 1979; Lawrence and Dorning, 1980), but this problem did not have a reference solution until now. The CUBBOX results (Langenbuch et. al., 1977) with mesh size 20 cm and time step 0.125 s are usually considered as a reference. These results, given in Fig. 5, contain average reactor power density and local power densities at the four core locations throughout the transient.

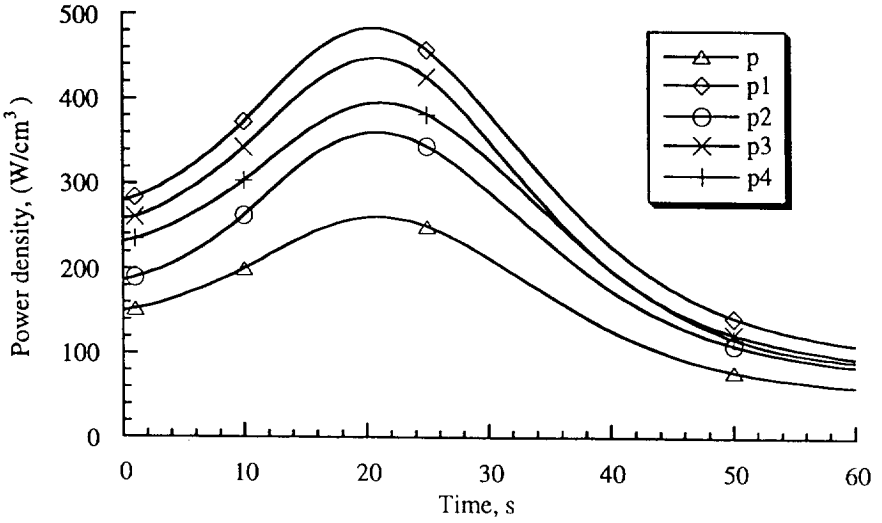

Fig. 5 CUBBOX solution of the LMW neutron kinetics (6x6x10, Δt=0.125 s).

The comparison of SKETCH results with different mesh sizes and CUBBOX 20-cm mesh-size results of the initial steady-state reactor model allows us to conclude that the CUBBOX calculation with 20 cm mesh size yields a level of accuracy comparable to the finite-difference SKETCH calculations using from 5 to 10-cm mesh size. Hence, 5 and 10-cm mesh sizes were chosen for the SKETCH calculations of the transient. Time step size of the SKETCH calculations was the same as for the CUBBOX calculation and was equal to 0.125 s. The given tolerance ζ was $5x10^{-4}$. The iteration matrix changes during the transient, so the adaptive Chebyshev procedure was used for improving the initial estimate of the iteration parameters for the CSA and the CSI methods. The new estimate was not recalculated while the power of Chebyshev polynomial was less than 5 and the damping factor F=0.65 was used for the calculations. The initial estimate of the second eigenvalue of the matrix $\tilde{\mathbf{B}}$ was equal to 0.90 and 0.94 for 10- and 5-cm mesh-size calculations, respectively; the initial estimate of the first eigenvalue for the CSI method was equal to 0.99. The comparison of convergence behaviors of the methods are given in Fig. 6 (a), (b) at the time moment 1.125 s for the mesh sizes 10 and 5 cm respectively. Presented results show that the convergence of the CSA method is again much faster than the convergence of the CSI method. The average reactor power density obtained by the SKETCH code, their deviations from the CUBBOX solution and the number of outer iterations of CSA, CSI and MFSI methods are presented in Tables 2,3 for 10- and 5-cm mesh size SKETCH calculations respectively. The number of outer iterations of the CSA method does not practically change during the transient and the average number is equal to 9 iterations for mesh size 10 cm and 12 iterations for mesh size 5 cm. The obtained results show that the CSA method is about 3 times faster than the CSI method and even the MFSI method is competitive with the CSI method. Comparing the number of iterations at the first time step (time = 0.125 s) and at the time moment 1 s we can conclude that the "optimal" iterative approximation (35) decreases the number of outer iterations of the CSA and MFSI methods 1.5-3 times and significantly increases the efficiency of these methods for transient calculations.

The comparisons of SKETCH results obtained by using the CSA method and CUBBOX results with respect to local power densities are shown in Fig. 7. The analysis of the comparisons shows that CUBBOX results are not bounded by 5 and 10 cm SKETCH results as they were for steady-state calculations. This different time behavior of CUBBOX and SKETCH solutions may be due to the different methods of time integration implemented in CUBBOX and SKETCH codes. In order to verify this assumption the additional comparison of the solution obtained by QUANDRY (Smith, 1979)[1] and NGFM (Lawrence and Dorning, 1980) codes with CUBBOX results was performed. Both these codes use nodal methods of spatial approximation and fully-implicit schemes as the time integration method and have the same order of space-time discretization error as CUBBOX code. The derivations of the average reactor power densities obtained by SKETCH, QUANDRY and NGFM codes from the CUBBOX results are presented in Fig. 8. The comparison shows that the deviations of the SKETCH, QUANDRY and NGFM results from the CUBBOX solution have a similar time behavior and confirms the assumption that the deviations between the SKETCH and CUBBOX results are mainly due to the different time integration methods in SKETCH and CUBBOX codes.

CPU time of the LMW benchmark problem calculations can be estimated from the expression

$$\text{Time} = \Omega \text{x(Number of mesh points)x(Number of time steps)x}$$
$$\text{(Average number of outer iterations per time step)}, \quad \text{[seconds]};$$

where the parameter Ω is equal to $1.9x10^{-4}$ on the DEC 3000 workstation. For example, calculations using the CSA method with mesh sizes 10 and 5 cm and time step size 0.125 s (2 neutron energy groups, 480 time steps, 2340 and 18720 mesh points) require about 30 and 340 minutes. It's 4 and 43 seconds per time step, respectively.

[1] QUANDRY results of the LMW problem was taken from (Chao and Huang, 1989).

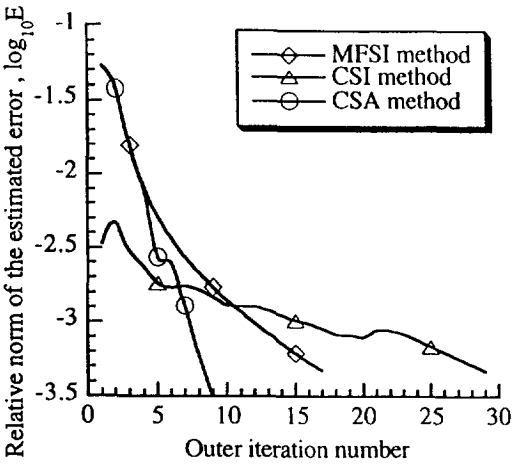

Fig. 6 (a) Convergence behavior of the MFSI, CSI and CSA methods for the LMW benchmark problem (time=1.125 s, Δt=0.125 s, 11x11x20).

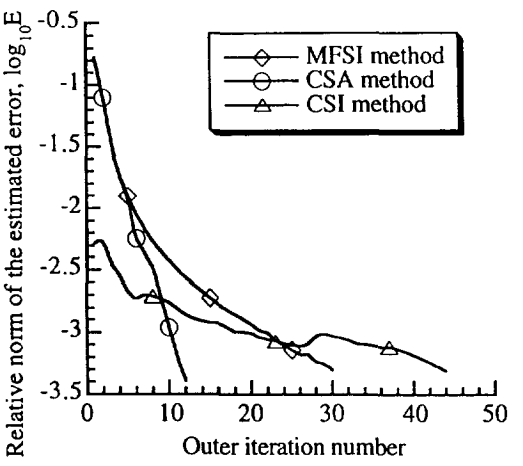

Fig. 6 (b) Convergence behavior of the MFSI, CSI and CSA methods for the LMW benchmark problem (time=1.125 s, Δt=0.125 s, 22x22x40).

Table 2. Solution of the Langenbuch-Maurer-Werner benchmark problem obtained by computer code SKETCH (11x11x20, Dt=0.125 s) using the MFSI, CSI and CSA iteration methods and the number of outer iterations.

Time, sec	Modified Fission Source Iteration (MFSI) method		Chebyshev Semi-Iterative (CSI) method		Chebyshev Semi-Analytical (CSA) method	
	Average power (deviat. from CUBBOX, %)	Number of outer iterations	Average power (deviat. from CUBBOX, %)	Number of outer iterations	Average power (deviat. from CUBBOX, %)	Number of outer iterations
0.125	150.2 (-)	50	150.2 (-)	19	150.2 (-)	16
1.0	152.4 (-0.1)	18	152.4 (-0.2)	30	152.5 (-0.1)	10
2.0	155.6 (0.0)	18	155.6 (-0.1)	31	155.6 (0.0)	10
5.0	168.6 (-0.1)	21	168.4 (-0.2)	36	168.6 (-0.1)	10
10.0	200.2 (0.0)	22	200.0 (-0.1)	39	200.2 (0.0)	10
15.0	234.7 (-1.5)	17	234.3 (-1.7)	36	234.6 (-1.6)	10
20.0	254.4 (-2.3)	20	253.8 (-2.6)	18	254.3 (-2.4)	10
25.0	242.5 (-3.0)	35	242.4 (-3.1)	35	242.4 (-3.1)	11
30.0	205.4 (-3.9)	33	205.3 (-3.9)	33	205.3 (-3.9)	11
40.0	122.7 (-3.8)	27	122.7 (-3.7)	32	122.7 (-3.8)	10
50.0	76.8 (-2.3)	20	76.8 (-2.2)	24	76.8 (-2.3)	7
60.0	59.2 (-1.8)	10	59.2 (-1.8)	22	59.2 (-1.8)	5
	Average number of outer iterations	**23**	Average number of outer iterations	**30**	Average number of outer iterations	**9**

Table 3. Solution of the Langenbuch-Maurer-Werner benchmark problem obtained by computer code SKETCH (22x22x40, Dt=0.125 s) using the MFSI, CSI and CSA iteration methods and the number of outer iterations.

Time, sec	Modified Fission Source Iteration (MFSI) method		Chebyshev Semi-Iterative (CSI) method		Chebyshev Semi-Analytical (CSA) method	
	Average power (deviat. from CUBBOX, %)	Number of outer iterations	Average power (deviat. from CUBBOX, %)	Number of outer iterations	Average power (deviat. from CUBBOX, %)	Number of outer iterations
0.125	150.3 (-)	90	150.1(-)	16	150.3(-)	21
1.0	152.5 (-0.1)	31	152.5 (-0.1)	43	152.5 (0.1)	13
2.0	155.8 (0.1)	31	155.8 (0.1)	44	156.0 (0.3)	13
5.0	169.3 (0.3)	37	169.1 (0.2)	48	169.3 (0.6)	13
10.0	201.7 (0.8)	40	201.4 (0.6)	51	201.6 (0.9)	13
15.0	238.1 (-0.1)	29	237.7 (-0.3)	55	238.2 (0.1)	12
20.0	258.2 (-0.9)	34	257.5 (-1.1)	16	258.4 (-0.5)	13
25.0	245.9 (-1.7)	60	245.6 (-1.8)	46	246.0 (-1.6)	14
30.0	206.7 (-3.2)	65	206.7 (-3.2)	48	206.6 (-3.1)	14
40.0	121.5 (-4.7)	55	121.6 (-4.6)	43	121.5 (-4.4)	14
50.0	75.3 (-4.1)	34	75.4 (-4.1)	32	75.4 (-3.9)	11
60.0	57.9 (-4.1)	15	57.9 (-4.1)	30	57.8 (-3.9)	7
	Average number of outer iterations	41	Average number of outer iterations	41	Average number of outer iterations	12

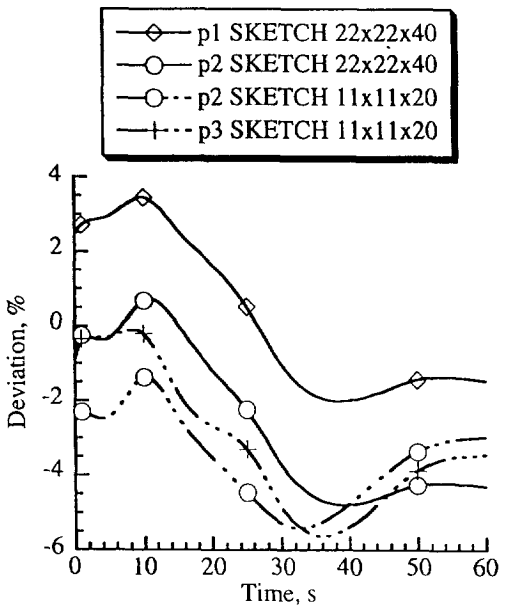

Fig. 7 Maximum deviations of the local power densities obtained by SKETCH code (11x11x20 and 22x22x40, Δt=0.125 s) from the CUBBOX results (6x6x10, Δt=0.125 s).

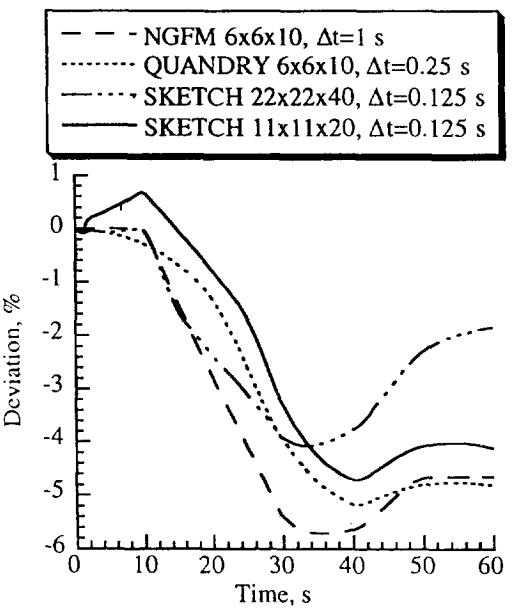

Fig. 8 Deviations of the average power density obtained by NGFM, QUANDRY and SKETCH codes from the CUBBOX results (6x6x10, Δt=0.125 s).

IX. CONCLUSIONS

The Chebyshev semi-analytical method has been developed for the solution of the space-dependent neutron kinetics equations. A Chebyshev polynomials sequence is chosen to optimize the residual vector convergence to the eigenvector of the iteration matrix. When the convergence is attained, the "exact" solution is obtained by adding the error vector to the approximate solution. The convergence rate of the CSA method is determined by the second eigenvalue of the iteration matrix. Convergence of the CSA method is always faster than convergence of the Chebyshev semi-iterative method and the relative effectiveness of the CSA method is determined by the dominance ratio of the iteration matrix. A priori and adaptive procedures have been developed for the estimate of the second eigenvalue of the iteration matrix which determines the optimal iteration parameters of the Chebyshev semi-analytical method. The efficiency of the Chebyshev semi-analytical method during transient calculations can be significantly increased using the proposed "optimal" initial approximation.

The acceleration procedure was implemented in the 3D neutron kinetics code SKETCH and a set of neutron kinetics benchmark problems was calculated. The results of benchmark problem calculations have shown that the convergence of the CSA method is significantly faster than that of the CSI method and the number of iterations of the CSA method is 2-5 times less than that of the CSI method. Relative efficiency of the CSA method has increased with an increase in time step sizes.

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