

Application of accelerated convergence techniques  
to the neutron diffusion-nodal model

by

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## I. INTRODUCTION

In the nuclear power industry, the need of a fast and accurate method to calculate the power distribution and flux profiles is very important. This is due to the increasing complexity of the reactor core and the economic emphasis on operational optimization.

Historically, finite difference methods were developed to solve this problem. However, as the situation becomes more and more complicated, especially in three-dimensional problems, the finite difference methods are too time consuming. For example, in a typical power reactor calculation, these calculations need prohibitive computing time (hours CPU time) and computer memory (thousands Kbyte), also, there are problems of data management and data retrieval associated with the use of these methods.

The nodal model techniques first developed in the computer code FLARE [1], were designed to solve the problem with less cost and still yield acceptable results for many reactor problems. These techniques generally use averaged neutronic properties over an assembly node to calculate average power distributions. Another approach A Polynomial Fitting Technique, has proven to be quite a good method on the basis of calculation precision [2]. However, there are intrinsic computational problems involved

in the method, numerical stability and convergence behavior exhibit some problems. This research was conducted to investigate the mathematical properties of the method and to find some techniques to speed the convergence rate; therefore, these new efficient techniques can be used in reactor applications.



## II. THE THEORY OF NEUTRON DIFFUSION NODAL MODEL

### A. The Discrete-Energy Group Diffusion Equation [3, 4]

The discrete-energy group neutron diffusion equation is given by

$$\begin{aligned}
 -D_{\gamma,g} \nabla^2 \phi_{\gamma,g} + [\Sigma_{a,\gamma,g} + \Sigma_{s,\gamma,g \rightarrow n} + D_{\gamma,g} B_g^2] \phi_{\gamma,g} \\
 = \sum_n [\Sigma_{s,\gamma,n \rightarrow g} + \frac{1}{K_{\text{eff}}} \chi_{\gamma,g} (\nu \Sigma)_{f,\gamma,n}] \phi_{\gamma,n}
 \end{aligned}$$

where

$\nabla^2$  = the Laplacian geometric operator,  $\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$

in two-dimensional rectangular geometry

$\phi_{\gamma,g}$  = the neutron flux at location  $\gamma$  and in energy group  $g$ , n/sec-cm<sup>2</sup>

$\Sigma_{a,\gamma,g}$  = the macroscopic absorption cross section cm<sup>-1</sup>

$\Sigma_{s,\gamma,g \rightarrow n}$  = the macroscopic scattering cross section from energy group  $g$  to energy group  $n$ , cm<sup>-1</sup>

$D_{\gamma,g}$  = the diffusion coefficient, cm

$B_g^2$  = the transverse buckling term to account for the effect of the leakage in the direction not treated explicitly, cm<sup>-2</sup>

$\nu \Sigma_{f,\gamma,g}$  = the macroscopic production cross section, cm<sup>-1</sup>

$\chi_{\gamma,g}$  = the fission spectrum function,  $\sum_g \chi_{\gamma,g} = 1.0$

$K_{\text{eff}}$  = the effective multiplication factor

$\gamma$  = space location

$g$  = energy group

In this research, the cross section data were obtained from a fine mesh diffusion theory calculation so that results can be compared to these more accurate calculations [5].

The following sections give a brief introduction to the new mathematical method for solving this equation.

### B. Neutron Diffusion-Nodal Model Concept

The basic idea of this method is to present the flux distribution over fuel assemblies in terms of a polynomial (Fig. 1, Fig. 2)

$$\phi(x) = a + bx + cy + dx^2 + ey^2 \quad (2-1)$$

The neutron balance equation can be solved easily by a simple evaluation, e.g., the leakage term becomes

$$\begin{aligned} L = & \int_{-\frac{\Delta}{2}}^{\frac{\Delta}{2}} D \frac{\partial \phi}{\partial x} \Big|_{x=\frac{\Delta}{2}} dy + \int_{-\frac{\Delta}{2}}^{\frac{\Delta}{2}} D \frac{\partial \phi}{\partial y} \Big|_{y=\frac{\Delta}{2}} dx \\ & + \int_{-\frac{\Delta}{2}}^{\frac{\Delta}{2}} D \frac{\partial \phi}{\partial x} \Big|_{x=-\frac{\Delta}{2}} dy + \int_{-\frac{\Delta}{2}}^{\frac{\Delta}{2}} D \frac{\partial \phi}{\partial y} \Big|_{y=-\frac{\Delta}{2}} dx \end{aligned} \quad (2-2)$$

the integration can be evaluated over the fuel nodes easily which in other methods the calculation of leakage term can be very complicated. Similarly, much additional useful information can be obtained as long as the coefficients have been

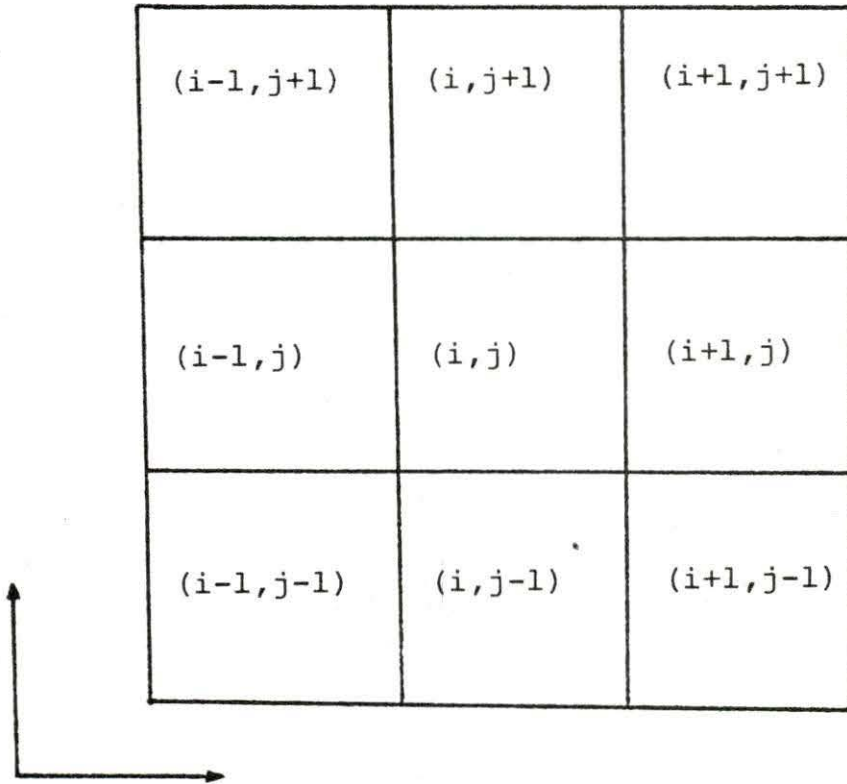


Figure 1. Fuel arrangement geometry

evaluated.

The advantage of a polynomial representation becomes obvious because the manipulation of a polynomial function is much easier and simpler when compared to the manipulation of a set of discrete point values. However, the determination of the coefficients of the polynomial becomes the major concern of this method. This presents other kinds of problems and difficulties.

### C. The Determination of the Coefficients

Assume that the flux distribution over the fuel assemblies are known, then one can apply a simple mathematical technique and the coefficients can be solved directly. One can determine the averaged flux over fuel assembly (i,j) to be (see Fig. 1)

$$\begin{aligned}\bar{\phi}_{i,j} &= \frac{1}{\Delta^2} \int_{-\frac{\Delta}{2}}^{\frac{\Delta}{2}} dx \int_{-\frac{\Delta}{2}}^{\frac{\Delta}{2}} dy \phi(x,y) \\ &= \frac{1}{\Delta^2} \int_{-\frac{\Delta}{2}}^{\frac{\Delta}{2}} (ax + \frac{bx^2}{2} + cyx + \frac{d}{3}x^3 + exy^2) dy \\ &= a + (d+e) \frac{\Delta^2}{12}\end{aligned}\tag{2-3}$$

One can assume the flux distribution in node (i,j) can be extended into the surrounding assemblies. The averaged fluxes of the neighboring fuel assemblies are:

$$\bar{\phi}_{i+1,j} = a + \Delta b + (13d+e)\frac{\Delta^2}{12} \quad (2-4)$$

$$\bar{\phi}_{i-1,j} = a - \Delta b + (13d+e)\frac{\Delta^2}{12} \quad (2-5)$$

$$\bar{\phi}_{i,j+1} = a + \Delta c + (d+13e)\frac{\Delta^2}{12} \quad (2-6)$$

$$\bar{\phi}_{i,j-1} = a - \Delta c + (d+13e)\frac{\Delta^2}{12} \quad (2-7)$$

The coefficients from Equations (2-3) to (2-7) can be solved:

$$\begin{aligned} a &= \frac{28\phi_{i,j} - \phi_{i+1,j} - \phi_{i-1,j} - \phi_{i,j+1} - \phi_{i,j-1}}{24} \\ b &= \frac{\phi_{i+1,j} - \phi_{i-1,j}}{2\Delta^2} \\ c &= \frac{\phi_{i,j+1} - \phi_{i,j-1}}{2\Delta^2} \\ d &= \frac{\phi_{i+1,j} - 2\phi_{i,j} + \phi_{i-1,j}}{2\Delta^2} \\ e &= \frac{\phi_{i,j+1} - 2\phi_{i,j} + \phi_{i,j-1}}{2\Delta^2} \end{aligned} \quad (2-8)$$

Equations (2-3) to (2-8) give the relationship between the flux distribution, the average fluxes and the coefficients.

#### D. The Partial Fluxes

The purpose of introducing the idea of the partial flux is to take the space coupling effect into consideration. Since the diffusion coefficients are almost the same in the neighboring fuel assemblies, one can make the assumption that the flux for a node  $(i,j)$  will be continuous across

the boundary at least in the partial regions of the surrounding nodes.

In Fig. 2, the average partial flux at the right side can be evaluated as:

$$\begin{aligned}
 \psi_{i,j}^Y &= \frac{1}{A_Y} \int_{-\frac{\Delta}{2}}^{\frac{\Delta}{2}} \int_{\frac{\delta}{2}}^{\frac{\Delta}{2}} dx \phi(x, y) \\
 &= \frac{1}{\Delta \left( \frac{\Delta}{2} - \frac{\delta}{2} \right)} \int_{-\frac{\Delta}{2}}^{\frac{\Delta}{2}} \int_{\frac{\delta}{2}}^{\frac{\Delta}{2}} dx (a + bx + cy + dx^2 + ey^2) \\
 &= a + \frac{b}{4} \Delta \left( 1 + \frac{\delta}{\Delta} \right) + \frac{e}{12} \Delta^2 \left( 1 + \frac{\delta}{\Delta} + \frac{\delta^2}{\Delta^2} \right) + \frac{e}{12} \Delta^2 \quad (2-9)
 \end{aligned}$$

Similarly, the average partial fluxes at the other sides are:

$$\psi_t = a + \frac{c}{4} \Delta \left( 1 + \frac{\delta}{\Delta} \right) + \frac{e}{12} \Delta^2 \left( 1 + \frac{\delta}{\Delta} + \frac{\delta^2}{\Delta^2} \right) + \frac{d}{12} \Delta^2 \quad (2-10)$$

$$\psi_e = a - \frac{b}{4} \Delta \left( 1 + \frac{\delta}{\Delta} \right) + \frac{d}{12} \Delta^2 \left( 1 + \frac{\delta}{\Delta} + \frac{\Delta^2}{\Delta^2} \right) + \frac{e}{12} \Delta^2 \quad (2-11)$$

$$\psi_b = a - \frac{c}{4} \Delta \left( 1 + \frac{\delta}{\Delta} \right) + \frac{e}{12} \Delta^2 \left( 1 + \frac{\delta}{\Delta} + \frac{\Delta^2}{\Delta^2} \right) + \frac{e}{12} \Delta^2 \quad (2-12)$$

Now, extend the partial flux into surrounding regions, apply the definition of averaged flux and reference to Fig. 3.

$$\begin{aligned}
 \psi_{\ell, i+1, j} &= \frac{1}{A_Y} \int_{-\frac{\Delta}{2}}^{\frac{\Delta}{2}} \int_{\frac{\Delta}{2}}^{\Delta - \frac{\delta}{2}} \phi(x, y) = a + \frac{b}{4} \Delta \left( 3 - \frac{\delta}{\Delta} \right) \\
 &\quad + \frac{d}{12} \Delta^2 \left( 7 - 5 \frac{\delta}{\Delta} + \frac{\delta^2}{2\Delta^2} \right) + \frac{e}{12} \Delta^2 \quad (2-13)
 \end{aligned}$$

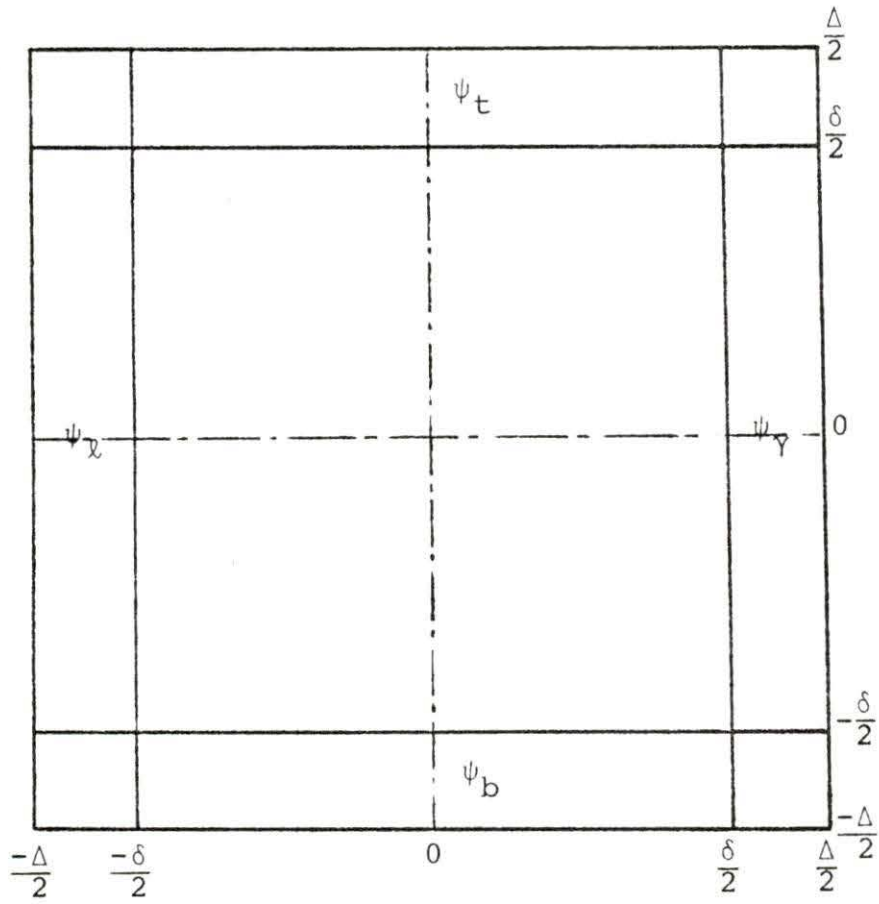


Figure 2. Partial flux concept for node  $i,j$

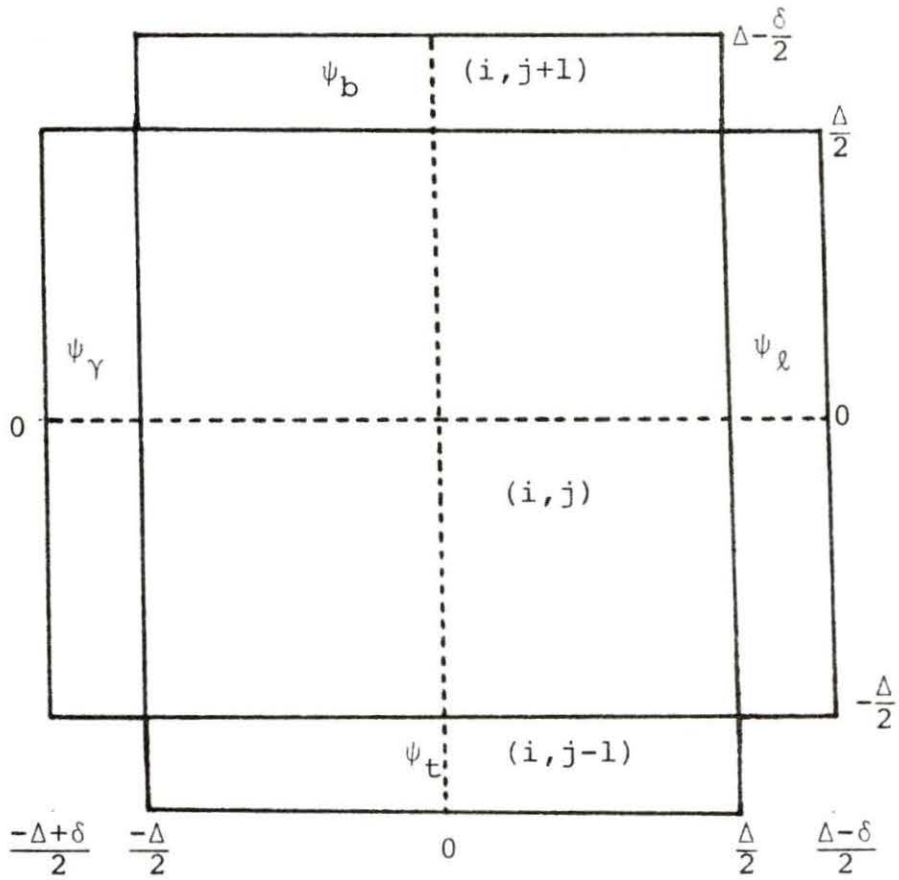


Figure 3. Extend partial flux into neighboring nodes



$$\psi_{b,i,j+1} = a + \frac{c}{4}\Delta(3-\frac{\delta}{\Delta}) + \frac{e}{12}\Delta^2(7-5\frac{\delta}{\Delta} + (\frac{\delta}{\Delta})^2) + \frac{d}{12}\Delta^2 \quad (2-14)$$

$$\psi_{\gamma,i-1,j} = a - \frac{b}{4}\Delta(3-\frac{\delta}{\Delta}) + \frac{d}{12}\Delta^2(7-5\frac{\delta}{\Delta} + (\frac{\delta}{\Delta})^2) + \frac{e}{12}\Delta^2 \quad (2-15)$$

$$\psi_{t,i,j-1} = a - \frac{c}{4}\Delta(3-\frac{\delta}{\Delta}) + \frac{e}{12}\Delta^2(7-5\frac{\delta}{\Delta} + (\frac{\delta}{\Delta})^2) + \frac{d}{12}\Delta^2 \quad (2-16)$$

The new coefficients based on these partial fluxes are:

$$a = \frac{2[8-5\frac{\delta}{\Delta} + (\frac{\delta}{\Delta})^2]\phi_{ij} - \psi_{\ell,i+1,j} - \psi_{\gamma,i-1,j} - \psi_{b,i,j+1} - \psi_{t,i,j-1}}{2[6-5\frac{\delta}{\Delta} + (\frac{\delta}{\Delta})^2]}$$

$$b = \frac{\psi_{\ell,i+1,j} - \psi_{\gamma,i-1,j}}{\frac{\Delta}{2}(3-\frac{\delta}{\Delta})}$$

$$c = \frac{\psi_{b,i,j+1} - \psi_{\gamma,i-1,j}}{\frac{\Delta}{2}(3-\frac{\delta}{\Delta})} \quad (2-17)$$

$$d = \frac{\psi_{\ell,i+1,j} - 2\phi_{i,j} + \psi_{\gamma,i-1,j}}{\frac{\Delta^2}{6}(6-5\frac{\delta}{\Delta} + (\frac{\delta}{\Delta})^2)}$$

$$e = \frac{\psi_{b,i,j+1} - 2\phi_{ij} + \psi_{t,i,j-1}}{\frac{\Delta^2}{6}(6-5\frac{\delta}{\Delta} + (\frac{\delta}{\Delta})^2)}$$

These new coefficients approximate the continuity of fluxes between the fuel assemblies.

## E. Assembly Average Bucklings

One big advantage of Diffusion-Nodal model over other methods is that it is easy to calculate the leakages between fuel assembly, refer to Fig. 4, the leakage from the right side of node  $(i,j)$  is equal the leakage from the left side of node  $(i+1,j)$

$$L_{\gamma} = - \int_{-\frac{\Delta}{2}}^{\frac{\Delta}{2}} D_{i,j} \left. \frac{\partial \phi}{\partial x} \right| dy = - \int_{-\frac{\Delta}{2}}^{\frac{\Delta}{2}} D_{i+1,j} \left. \frac{\partial \phi}{\partial x} \right| dy$$

However, these two will not be equal because of the polynomial approximation. Therefore, define

$$L_{\gamma} \equiv - \frac{[W_1 (D_{i,j} (b_{i,j} + \Delta d_{i,j}) \Delta) + W_2 (D_{i+1,j} (b_{i+1,j} - \Delta d_{i+1,j}) \Delta)]}{W_1 + W_2} \quad (2-18)$$

Here we introduce two weighting factors  $W_1, W_2$  to adjust the flux level to preserve the continuity of current over fuel assemblies. The leakage term for the other three directions are:

$$L_t = \left[ \frac{-W_1 (C_{i,j} + \Delta \ell_{i,j}) D_{i,j} + W_2 (C_{i,j+1} - \Delta \ell_{i,j+1}) D_{i,j+1}}{W_1 + W_2} \right] \Delta \quad (2-19)$$

$$L_{\ell} = \left[ \frac{W_1 (b_{i,j} - \Delta d_{i,j}) D_{i,j} + W_2 (b_{i-1,j} - \Delta d_{i-1,j}) D_{i-1,j}}{W_1 + W_2} \right] \Delta \quad (2-20)$$

$$L_b = \left[ \frac{W_1 (d_{ij} - \Delta \ell_{i,j}) D_{i,j} + W_2 (C_{i,j-1} - \Delta \ell_{i,j-1}) D_{i,j-1}}{W_1 + W_2} \right] \Delta \quad (2-21)$$

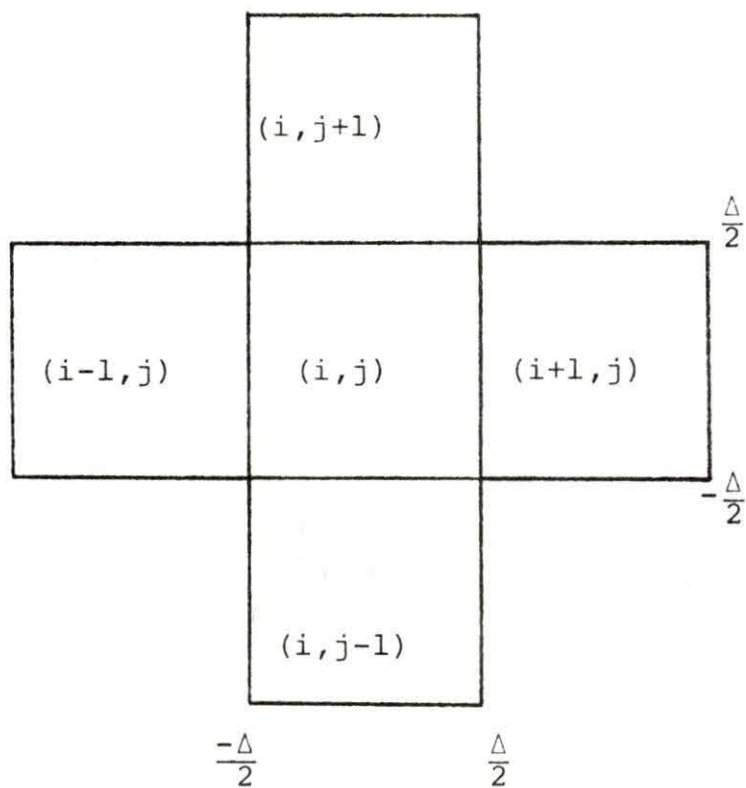


Figure 4. Nodes involved in the leakage calculation for node  $(i, j)$

from the physical definition of buckling: total leakage =

$$DV^2\bar{\phi} = DB^2\bar{\phi}$$

$$B_{i,j} = \frac{L_{\gamma} + L_t + L_{\ell} + L_b}{D_{i,j} \bar{\phi}_{i,j} \Delta^2} \quad (2-22)$$

#### F. The Calculation Procedure

The overall calculation procedure flowchart is illustrated in Fig. 5. The calculation starts with an initial flux guess and the partial fluxes are from these initial fluxes. Then the coefficients are calculated according to Eq. (2-17). The purpose of the mathematically averaged flux calculation is to insure that there is flux continuity between neighboring assemblies. A new set of coefficients is calculated again and then used to evaluate the leakages which in turn are used to calculate the bucklings. Finally, the new averaged fluxes can be obtained by simply solving the neutron balance equations. A new iteration begins by calculating new partial fluxes based upon the new fluxes just obtained. Iterations are repeated until the flux changes less than a preset tolerance criterion.

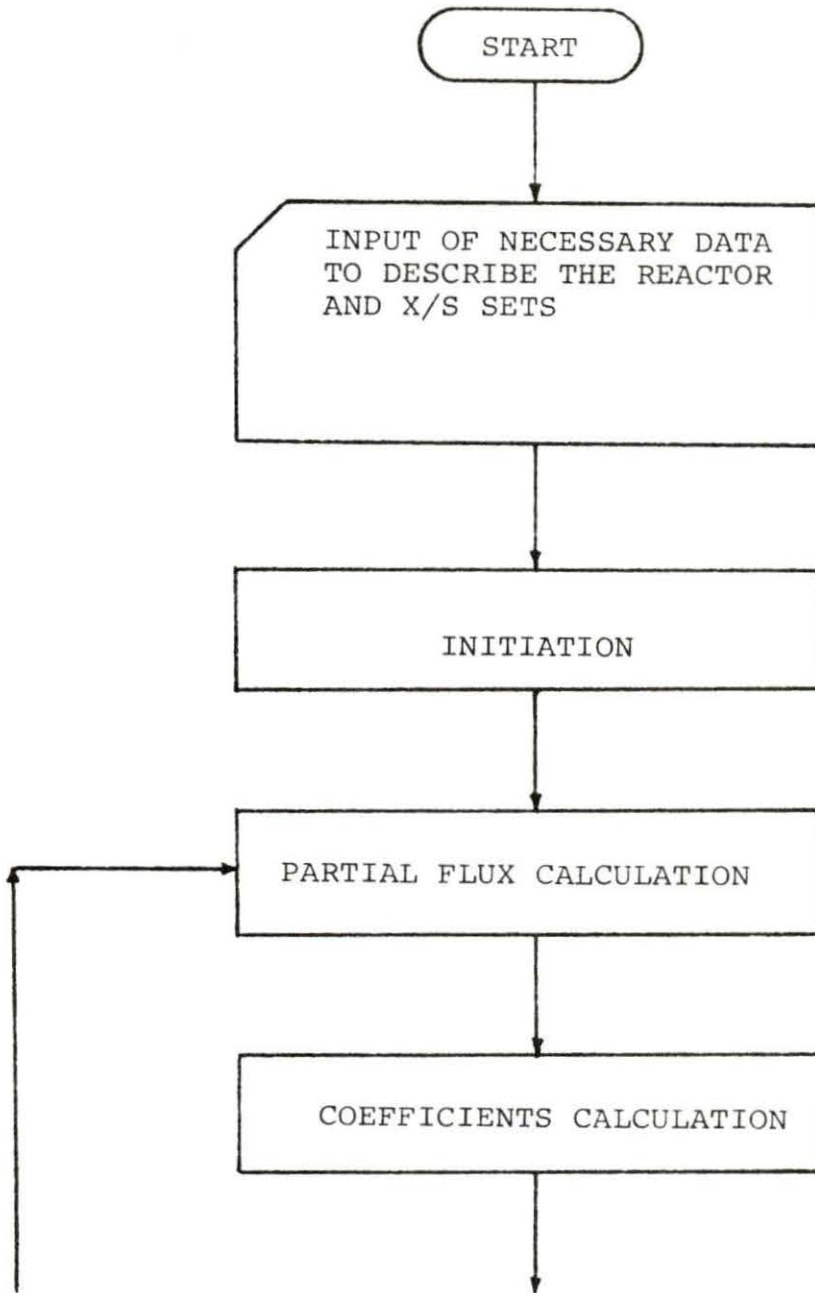


Figure 5. Calculation flowchart

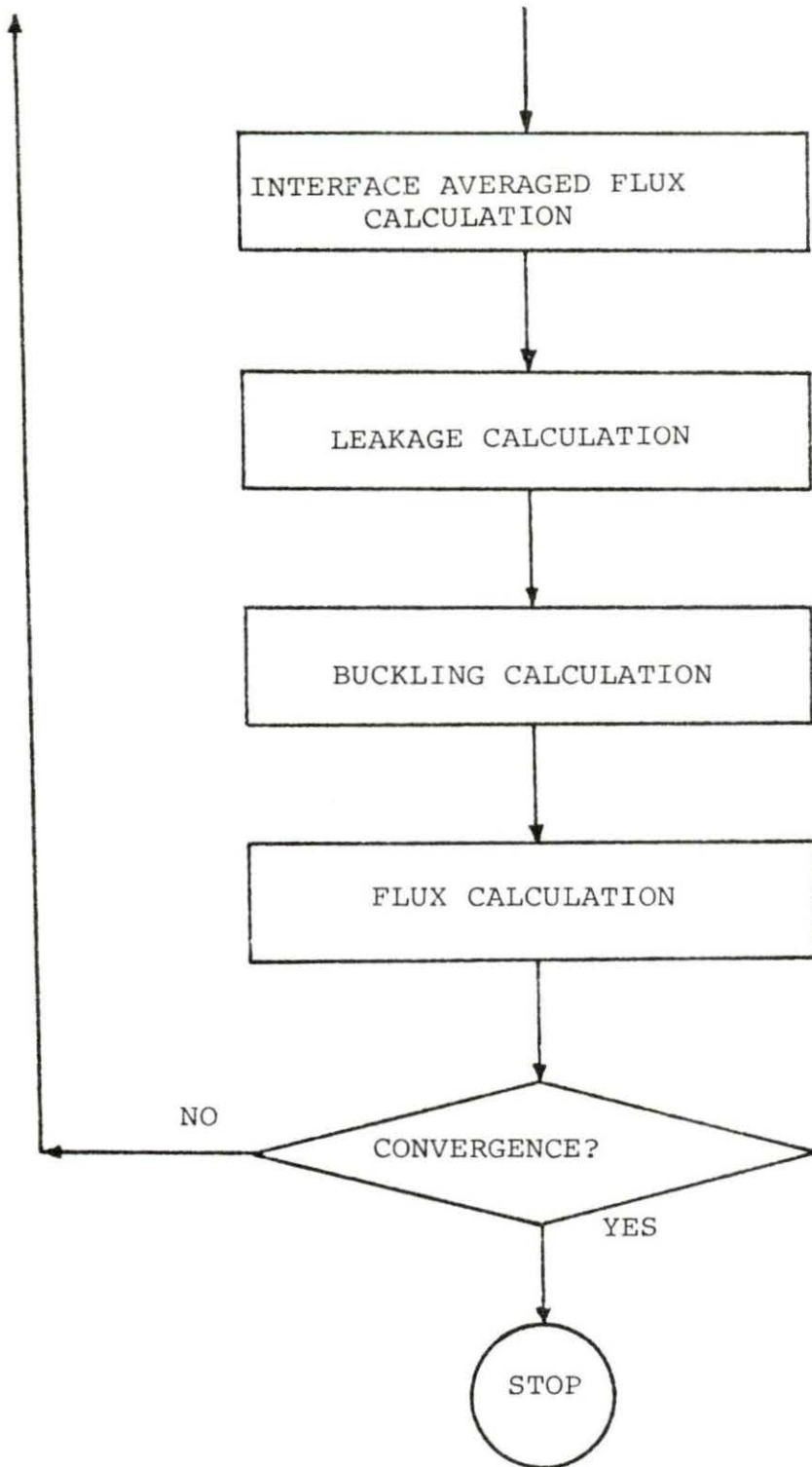


Figure 5 (Continued)

### III. THE THEORY OF ACCELERATING TECHNIQUES

#### A. The Acceleration of the Iterative Process

For a specific system of equations, if the solutions are obtained by an iterative process, then it is possible to ensure the convergence and also to improve the rate of convergence by applying some kind of mathematical techniques. These mathematical techniques vary from a simple extrapolation to some sophisticated matrix manipulations called "acceleration techniques."

Of most techniques being used for acceleration, the general principle is to split the iteration matrix into different forms. Following are some fundamental definitions and theories related to the convergence properties and accelerating mechanisms; these theories will be used frequently in the next chapter.

##### 1. General convergence theorems

Definition 3.1: [6] If  $X' \in \mathbb{R}^n$  is an approximation to the solution of the linear system defined by  $AX = b$ , the residual vector for  $X'$  with respect to this system is defined by  $\gamma = b - AX' = AX - AX' = A(X - X')$ .

The concept of residual vector will be used frequently as a measure of the closeness of the approximate solution to the exact solution.

Theorem 3.2: [6] If  $X'$  is an approximation to the solution of  $AX = b$  and  $A$  is a nonsingular matrix, then for any natural norm

$$\|X - X'\| \leq \|\gamma\| \|A^{-1}\| \quad (3-1)$$

and

$$\frac{\|X - X'\|}{\|X\|} \leq \|A\| \|A^{-1}\| \frac{\|\gamma\|}{\|b\|} \quad \text{provided } X \neq 0 \text{ and } b \neq 0, \quad (3-2)$$

where  $\gamma$  is the residual vector for  $X'$  with respect to the system  $AX=b$ .

Equations 3-1 and 3-2 imply that the quantities  $\|A^{-1}\|$  and  $\|A\| \|A^{-1}\|$  can be used to give an indication of the closeness between the residual and the accuracy of the approximation; also 3-2 shows the relative error  $\frac{\|X - X'\|}{\|X\|}$  is bounded by the product of  $(\|A\| \|A^{-1}\|)$ .

Theorem 3.3: [6] The sequence  $\{X^{\ell}\}_{\ell=0}^{\infty}$  defined by

$$X^{(\ell)} = AX^{(\ell-1)} + C \quad (3-3)$$

for each  $\ell > 1$  and  $C \neq 0$

converges to the vector  $X$  for any

$X^{(0)} \in \mathbb{R}^n$  if and only if  $\rho(A) < 1$ .

This theory explains the necessary condition for an iterative process to be convergent, no matter what the initial vector  $X^{(0)}$  is. Matrix  $A$  must be a convergent matrix,



From basic vector theory, a convergent matrix always has a spectral radius less than 1.

## 2. Rates of convergence

From Theorem 3-3, if  $\|A\| < 1$  for any matrix norm then the sequence  $\{X^{(l)}\}_{l=0}^{\infty}$  in Eq. (3-3) converges for any  $X^{(0)} \in \mathbb{R}^n$  to vector  $X \in \mathbb{R}^n$  and also the following error bounds hold

$$\|X - X^{(l)}\| \leq \|A\|^l \|X^{(0)} - X\| \quad (3-4)$$

$$\|X - X^{(l)}\| \leq \frac{\|A\|^l}{1 - \|A\|} \|X^{(1)} - X^{(0)}\| \quad (3-5)$$

again from basic vector theory [7]

$$\rho(A) \leq \|A\| \quad (3-6)$$

then (3-4) becomes

$$\|X - X^{(l)}\| \approx \rho(A)^l \|X^{(0)} - X\| \quad (3-7)$$

If  $\rho(A) < 1$  is satisfied and  $X^{(0)} = 0$  is to be used in an iterative technique to approximate  $X$  with relative error of at most  $10^{-t}$ , then from Eq. (3-7) the relative error after  $l$  iterations is approximately  $\rho(A)^l$ . So accuracy of  $10^{-t}$  is expected if

$$\rho(A)^l \leq 10^{-t}$$

or

$$l \geq \frac{t}{-\log_{10} \rho(A)} \quad (3-8)$$

Equation (3-8) says that the minimum number of iterations is inversely proportional to the quantity  $1/\log_{10} \rho(A)$ . We are thus led to the definition of the average rate of convergence by

$$R(A) = -\log \rho(A). \quad (3-9)$$

Equation (3-9) gives the essential principle to all kinds of accelerating techniques, namely, any mathematical technique to reduce the spectral radius  $\rho(A)$  will improve the rate of convergence. This is the theoretic foundation of all accelerating techniques.

#### B. Stationary Accelerating Techniques

In this work, the term "iteration" relates to the solution of the linear system:

$$AX = b \quad (3-10)$$

In general, the iteration process can be defined by the functions

$$\phi_0(A, b), \phi_1(X^{(0)}, A, b), \phi_2(X^{(0)}, X^{(1)}; A, b) \dots$$

$$\phi_k(X^{(0)}, X^{(1)}, \dots, X^{(\ell-1)}; A, b)$$

the sequence  $X^{(0)}, X^{(1)} \dots$  is defined by

$$X^{(0)} = \phi_0(A, b)$$

$$X^{(\ell+1)} = \phi_{\ell+1}(X^{(0)}, X^{(1)}, \dots, X^{(\ell)}; A, b) \quad (3-11)$$

If, for some integer  $s > 0$ ,  $\phi_\ell$  is independent of  $\ell$  for all  $\ell \geq s$ , then the method is said to be stationary. Otherwise it is nonstationary. A general form for a stationary iterative method is

$$X^{(\ell+1)} = GX^{(\ell)} + k \quad (3-12)$$

the corresponding form to Equation (3-11) is

$$X^{(\ell+1)} = \phi_1(X^\ell; A, b)$$

Assume we are solving the equation

$$AX = b$$

Split  $A$  into  $A \equiv N_0 - P_0$

With  $X^{(0)}$  arbitrary, then the iterative process is given by

$$N_0 X^{(\ell)} = P_0 X^{(\ell-1)} + k$$

and with  $M_0 = N_0^{-1} P_0$  the iteration becomes

$$X^{(\ell)} = M_0 X^{(\ell-1)} + g \quad (3-13)$$

where

$$g = N_0^{-1}b$$

Now we introduce the one parameter family of splittings

$$\begin{aligned} N(\alpha) &= (1+\alpha)N_0 \\ P(\alpha) &= (1+\alpha)N_0^{-A} = P_0 + \alpha N_0 \end{aligned} \quad (3-14)$$

in order that  $\det|N(\alpha)| \neq 0$ ,  $\alpha \neq -1$  is required. If the eigenvalues of  $M(\alpha) = N^{-1}(\alpha)P(\alpha)$  are denoted by  $\mu_i(\alpha)$   $i = 1, 2, \dots, n$

then

$$\mu_i(\alpha) = \frac{\lambda_i + \alpha}{1 + \alpha} \quad i = 1, 2, \dots, n \quad (3-15)$$

because

$$\lambda_i < 1, \quad \mu_i(\alpha) < \lambda_i$$

This means after the splitting operation, the rate of convergence should be improved (refer to Equation 3-9). After a detailed study of Eqs. (3-14) and (3-15), the information about how to choose the best value of  $\alpha$  can be obtained.

The results may be stated as

Theorem 3-4: [8] Let  $N_0$  and  $P_0$  be such that the eigenvalues  $\lambda_i$  of  $N_0^{-1}P_0$  are all real and satisfy

$$\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n < 1$$

Then the scheme (3) will converge for any  $\alpha$  such that

$$\alpha > \frac{1 + \lambda_1}{2} > 1.$$

Furthermore, the largest rate of convergence for these schemes is obtained when

$$\alpha \equiv \alpha^* = \frac{-\lambda_1 + \lambda_n}{2} \quad (3-16)$$

for which value  $[M(\alpha^*) = \text{Min}_{\alpha} \rho[M(\alpha)]]$

$$= \text{Min}(\text{Max}_{i=1}^n |\mu_i(\alpha)|)$$

$$= \frac{\lambda_n - \lambda_1}{2 - \lambda_1 - \lambda_n} < 1$$

Another theory also gives the optimal value which is based upon a different splitting expression:

Theorem 3.5: [9]

If A is positive definite and tridiagonal then the optimal choice of  $\omega$  for SOR method is

$$\omega = \frac{2}{1 + \sqrt{1 - \rho(A)^2}} \quad (3-17)$$

with this choice of  $\omega$ ,  $\rho(A) = \omega - 1$ .

Now the problem is how to calculate  $\omega_{\text{opt}}$ , this will be explained in detail in the next chapter.

### C. Nonstationary Accelerating Techniques

Instead of just using one single fixed accelerating parameter, a cyclically fixed sequence of acceleration parameters can be applied to the accelerating scheme which

has shown a more powerful effect on the speed of convergence.

Assume in each cycle, there are  $\gamma$  parameters being used, say,  $\alpha_1, \alpha_2, \dots, \alpha_\gamma$ , for  $i = 1, 2, \dots, \gamma$ . Define  $N(\alpha_i)$  and  $P(\alpha_i)$  as in (3-14) and the corresponding matrices  $M(\alpha_i)$  by

$$M(\alpha_i) = N^{-1}(\alpha_i)P(\alpha_i) = \frac{\alpha_i}{1+\alpha_i} I + \frac{1}{1+\alpha_i} M_0, \quad i=1, 2, \dots, \gamma \quad (3-18)$$

The iterations are defined as follows, with  $X^{(0)}$  arbitrary for  $\ell = 1, 2, \dots$

$$Y^{(\ell, 0)} = X^{(\ell-1)} \quad (3-19)$$

$$Y^{(\ell, s)} = M(\alpha_s)Y^{(\ell, s-1)} + N^{-1}(\alpha_s)f \quad s = 1, 2, \dots, \gamma \quad (3-20)$$

$$X^{(\ell)} = Y^{(\ell, \gamma)} \quad (3-21)$$

where  $\gamma$  vectors of 3-20 can be obtained by solving a linear system of the form

$$N(\alpha_s)Y^{(\ell, s)} = P(\alpha_s)Y^{(\ell, s-1)} + f \quad (3-22)$$

With this notation, one iteration requires the same number of computations as  $\gamma$  iterations in the ordinary acceleration scheme. The convergence rate can be analyzed by means of the equivalent formulation

$$X^{(\ell)} = M(\alpha_1, \alpha_2, \dots, \alpha_\gamma)X^{(\ell-1)} + g, \quad \ell = 1, 2, \dots, \quad (3-23)$$

From Eqs. 3-19, 3-20 and 3-21

$$M(\alpha_1, \alpha_2, \dots, \alpha_\gamma) = M(\alpha_1)M(\alpha_2) \dots M(\alpha_\gamma) \quad (3-24)$$

the eigenvalues of  $M(\alpha_1, \alpha_2, \dots, \alpha_\gamma)$  can be determined in terms of the eigenvalues  $\lambda_i$  of  $M_0$ , i.e.:

$$\mu_i(\alpha_1, \alpha_2, \dots, \alpha_\gamma) = \prod_{j=1}^{\gamma} \frac{\lambda_i + \alpha_j}{1 + \alpha_j} \quad (3-25)$$

It is an  $\gamma$ th degree polynomial

$$P_\gamma(\lambda) = \prod_{j=1}^{\gamma} \frac{\lambda + \alpha_j}{1 + \alpha_j} \quad (3-26)$$

then convergence is implied by

$$|P_\gamma(\lambda_i)| < 1 \quad \text{for } i = 1, 2, \dots, n,$$

If all the eigenvalues of  $M_0$  are real and lie in the interval

$$a \leq \lambda \leq b$$

the convergence is implied by  $|P_\gamma(\lambda)| < 1$ ,  $a \leq \lambda \leq b$ .

In this case, the fastest convergence can be expected for that polynomial which has the smallest absolute magnitude in the indicated interval. The Chebyshev polynomial [10] the property of "the least deviation from zero", so if the zeroes of the Chebyshev polynomial are used as the accelerating parameter, the fastest convergence speed should be observed.

#### IV. ITERATION BEHAVIOR OF NEUTRON DIFFUSION NODAL MODEL

##### A. Iteration Processes

There are four processes in the iteration procedure. These include the partial flux calculation, interface averaged flux (also called averaged flux) calculation, buckling calculation and assembly averaged flux (also called just flux) calculation.

The purpose of the partial flux calculation, as shown in Fig. 6, is to take the space correlation of neighboring nodes into the calculation so that the averaged fluxes  $\bar{\phi}_1, \bar{\phi}_2, \dots, \bar{\phi}_n$  can represent the actual situation more accurately. But in the calculation of the partial fluxes, the average flux value used was obtained from the last iteration. The whole computation becomes a nonlinear procedure and gives problems in convergence speed and stability behavior.

The mathematically averaged flux calculation is followed by the partial flux calculation which in turn uses the coefficient set derived from the partial fluxes. The new averaged fluxes are calculated so that the flux distribution will keep continuity over the fuel assembly interface as shown in Fig. 7. After the new averaged fluxes are obtained, the leakage term can be calculated by a simple evaluation of Eq. (2-28). The buckling term can be



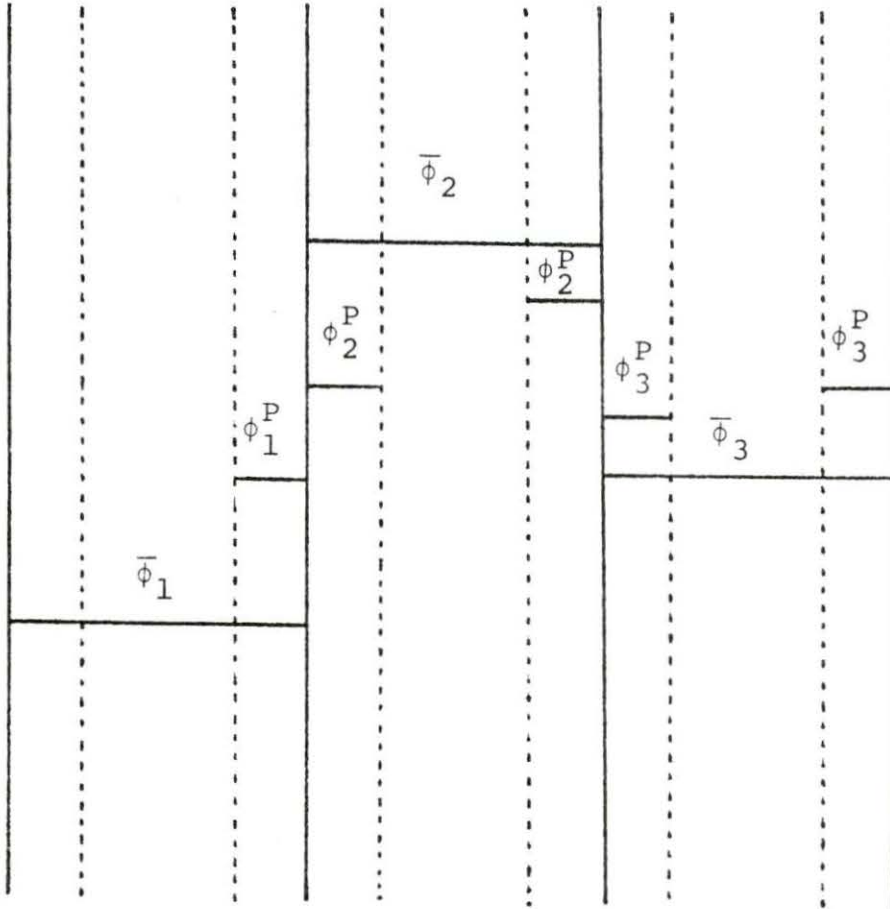


Figure 6. Partial flux calculation (one-dimensional view)

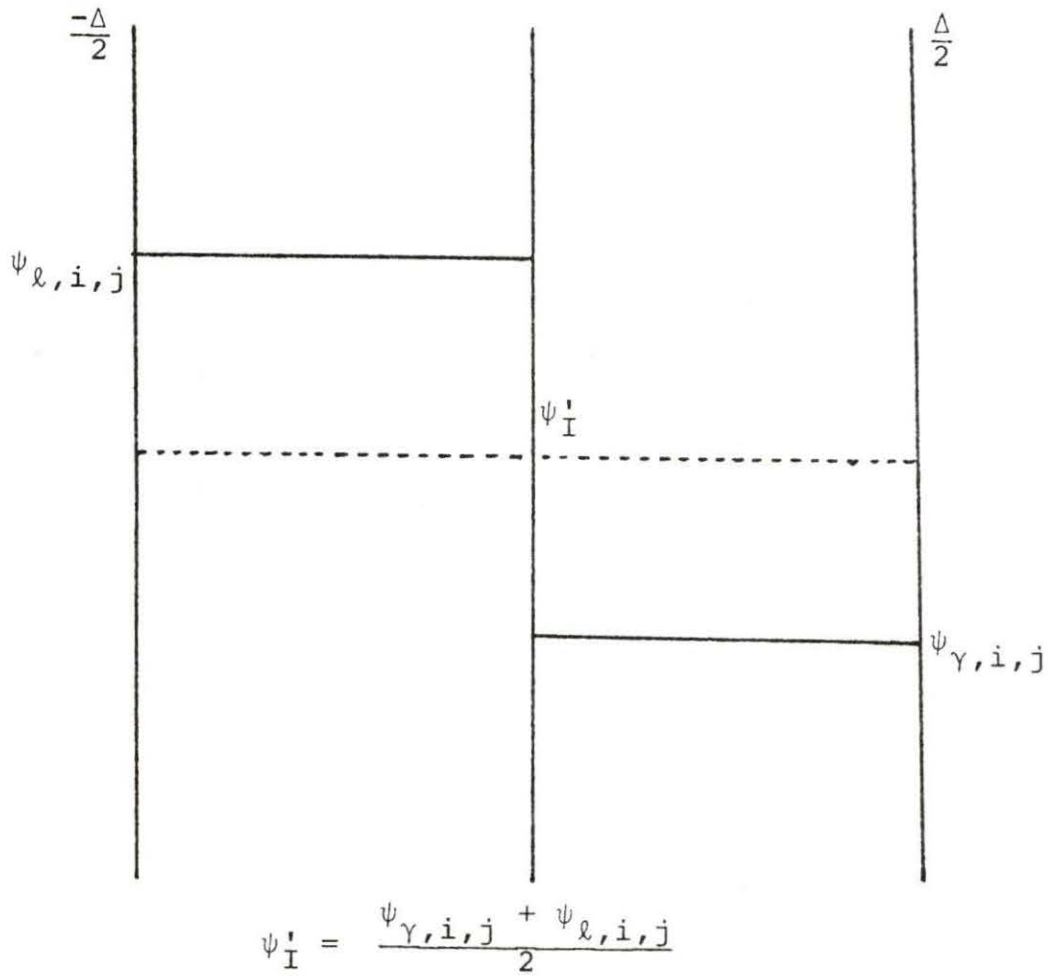


Figure 7. Interface average flux calculation (one-dimensional view)

computed in terms of the leakages, then the bucklings can be substituted into the two group flux equations

$$B_1^2 \phi_1 + \Sigma_{a1} \phi_1 + \Sigma_{1-2} \phi_1 = \nu \Sigma_{f1} \phi_1 + \nu \Sigma_{f2} \phi_2 \quad (4-1)$$

$$B_2^2 \phi_2 + a_2 \phi_2 = \Sigma_{1-2} \phi_1$$

and the average nodal fluxes can be determined. Then these new flux values will be used in the partial flux calculations in the next iteration.

#### B. Sensitivity Study

The purpose of the sensitivity study is to investigate the characteristics of each of the four relaxation processes and see which will have the most significant influence on the overall iteration behavior.

First, we found that without introducing any accelerating technique, the iteration process would not converge. After applying one standard technique we found that the iteration converged with the relaxation factor located in a specific range, i.e., it still will not converge with certain relaxation factors. Also, the convergence speed varied quite differently according to the different values of the relaxation factors.

The sensitivity study was carried out by fixing three of

the four relaxation factors and then by varying the value of the remaining one. The number of iterations needed to reach a preset convergence criterion was recorded. The procedure was repeated for every relaxation factor.

Figure 8 shows the effect of changing partial flux relaxation factor from 0.1 to 1.4. Figure 9 shows the effect of changing mathematical average flux relaxation factor from 0.1 to 1.4. Figure 10 shows the effect of changing the buckling relaxation factors from 0.1 to 1.2. Figure 11 shows the effect of changing the average flux relaxation factor from 0.1 to 1.7.

From these curves, it is very clear that one can easily conclude that buckling and assembly averaged flux relaxation factors have a stronger effect on the iteration behavior than the other two.

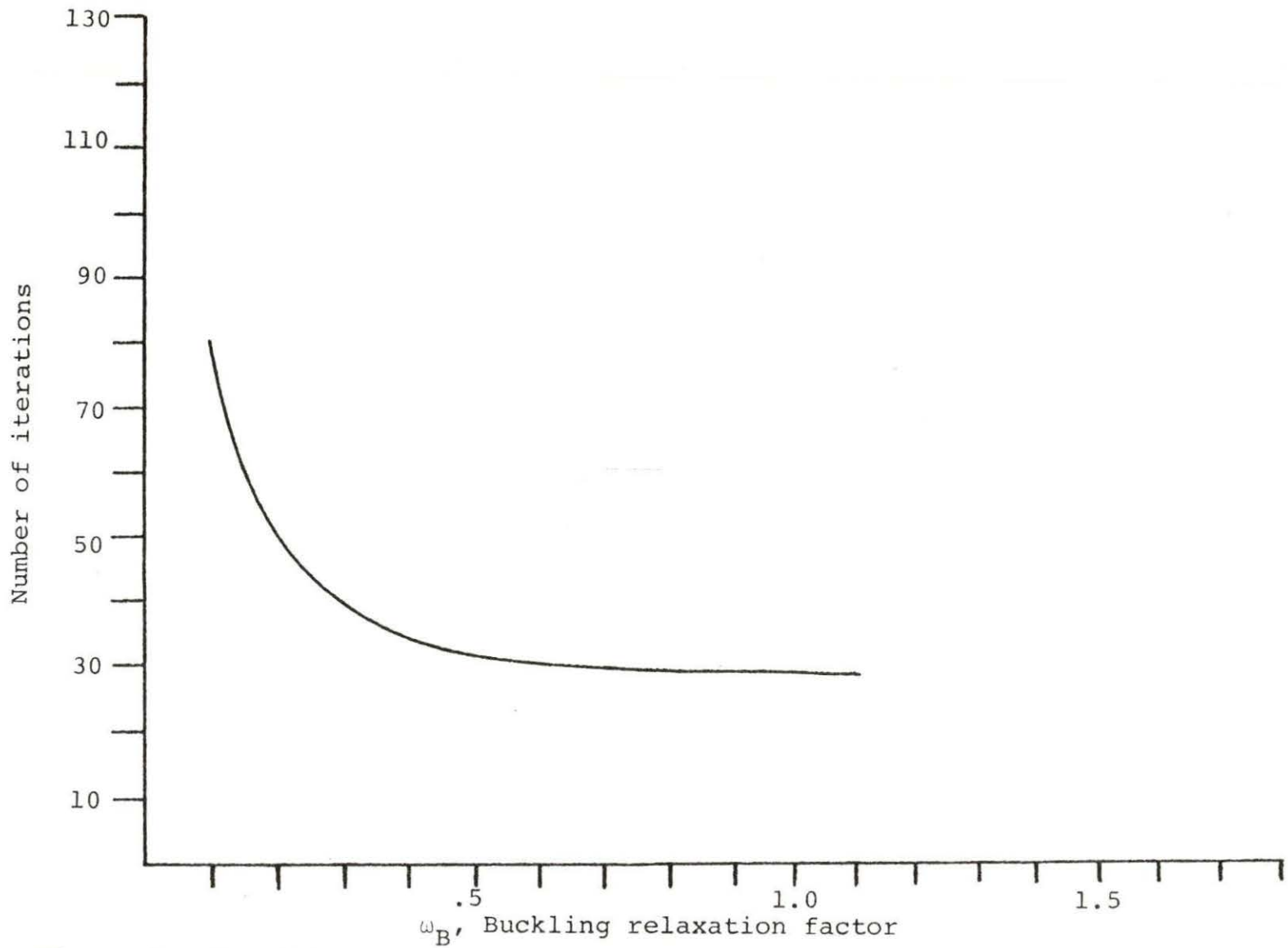


Figure 8. Sensitivity study for buckling relaxation factor

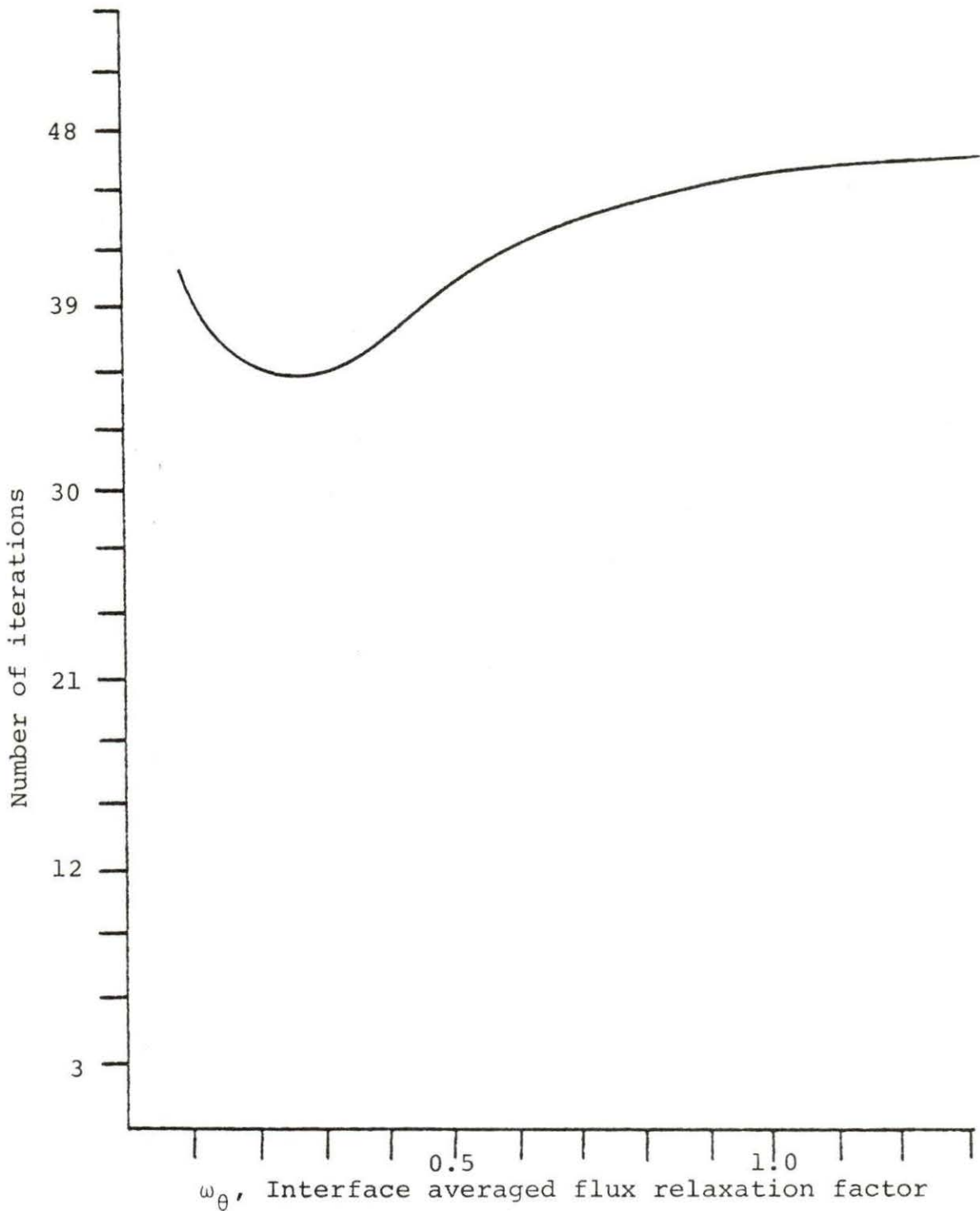


Figure 9. Sensitivity study for interface averaged flux relaxation factor

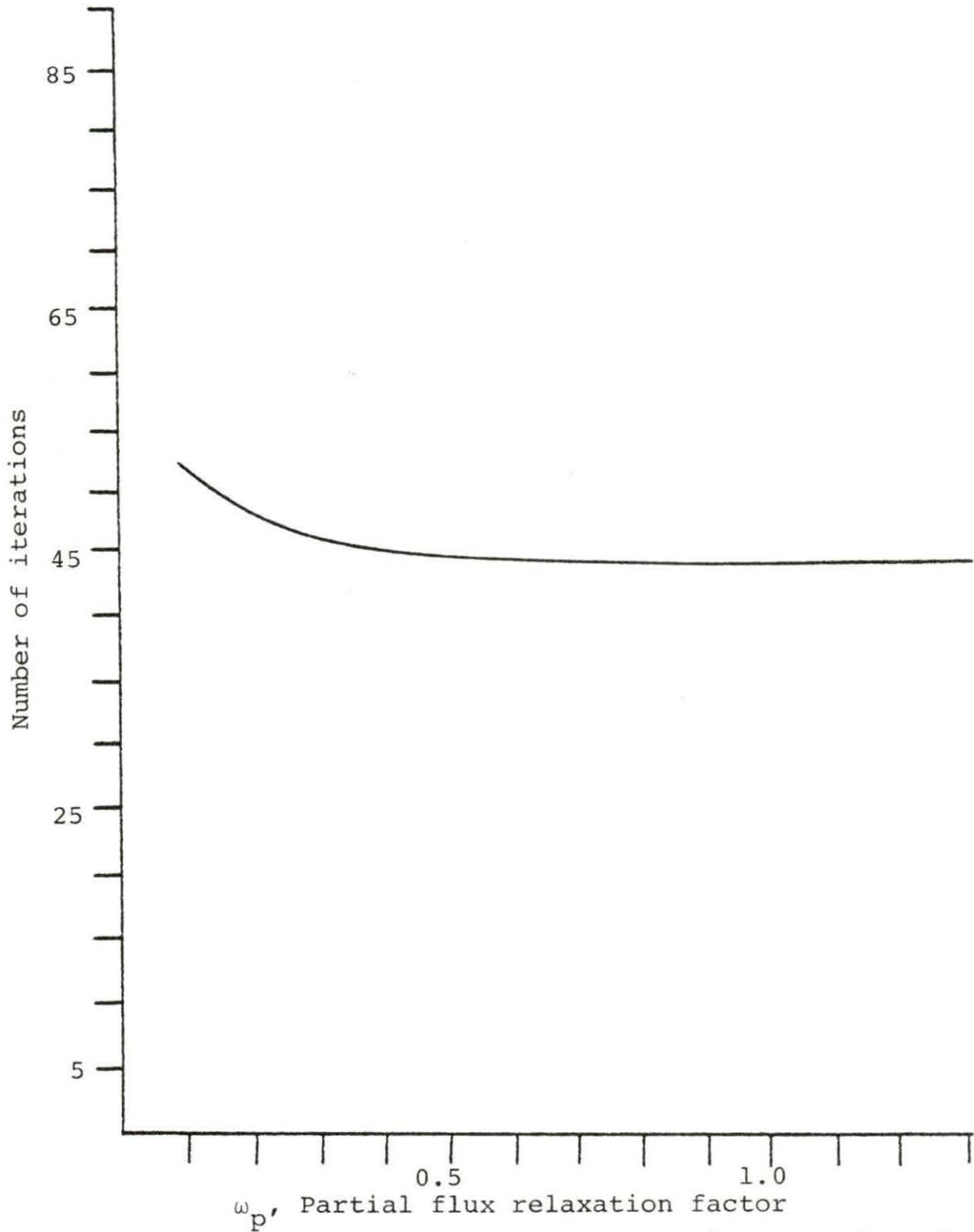


Figure 10. Sensitivity study for partial flux relaxation factor

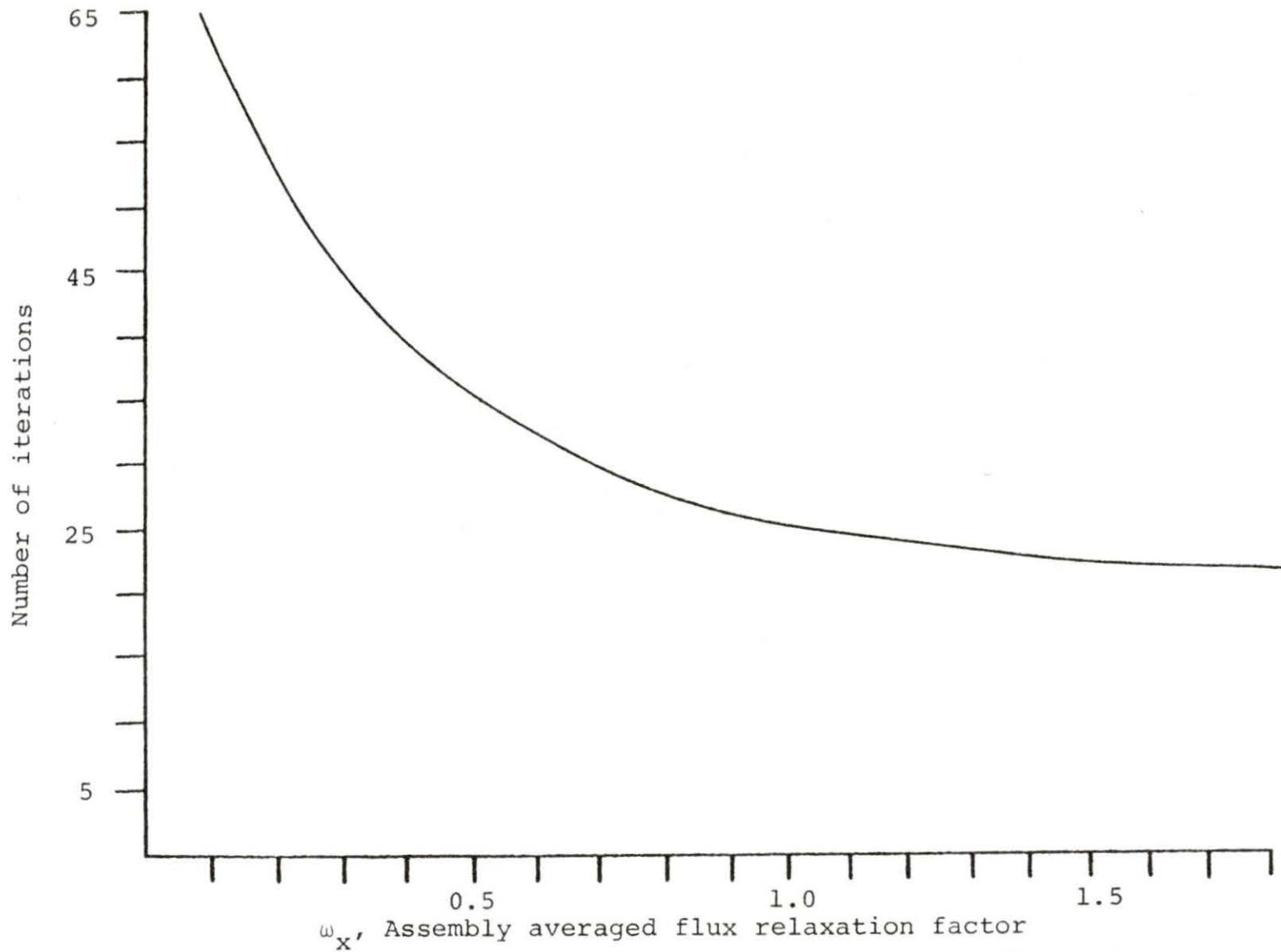


Figure 11. Sensitivity study for assembly averaged flux relaxation factor



## V. THE APPLICATION OF ACCELERATING TECHNIQUES

Both stationary and nonstationary accelerating techniques will be tried and compared in this chapter. A brief introduction about the test sample problem will be presented first.

### A. The Basic Data for the Sample Test Problem

The sample reactor chosen for this research was San Onofre I, a pressurized water reactor built by Westinghouse and operated by Southern California Edison Co.

Figure 12 shows the fuel assembly arrangement of the quarter core in two-dimensions. Table 1 lists the basic data of the reactor.

### B. Application of the Stationary Accelerating Techniques

The general form of linear stationary accelerating method is

$$\phi^{(n+1)} = G\phi^{(n)} + k \quad (5-1)$$

Depending upon the expression of  $G$ , there are more than 10 different accelerating techniques [11]. Among these methods, the Successive Overrelaxation (SOR) method is the most popular and most powerful one. So we will concentrate

H	6	7	8	9	10	11	12	13
J	14	15	16	17	18	19	20	21
K	22	23	24	25	26	27	28	
L	29	30	31	32	33	34	35	
M	36	37	38	39	40	41		
N	42	43	44	45	46			
P	47	48	49	50				
R	51	52						

Figure 12. Fuel assembly arrangement of the sample reactor

Table 1. Basic data of sample test reactor

---

Rated core heat output, MWe	3390
System pressure, psia	2250
Coolant flow, lb/h	$1.48 \times 10^8$
Coolant temperature, °F	
Nominal inlet	553
Nominal outlet	649.2
Full assemblies	
Rod pitch, in.	0.5063
Fuel weight, lbs	$223.9 \times 10^3$
Total weight	314867
Number of fuel assemblies	217

---

our effort in the application of the SOR technique to the Diffusion-Nodal model.

### 1. The SOR method

The iterative matrix for the SOR method in (5-1) is

$$G = (I - \omega L)^{-1} (\omega U + (1 - \omega)I) \quad (5-2)$$

a more usable form for SOR is

$$\phi^{(n+1)} = \omega \phi^* + (1 - \omega) \phi^{(n)} \quad (5-3)$$

or

$$\phi^{(n+1)} = \phi^{(n)} + \omega (\phi^* - \phi^{(n)})$$

where  $\phi^*$  is obtained from the Gauss-Seidel iterative method.

The most important procedure when using the SOR method is to determine the optimal relaxation factor  $\omega$ , which can be calculated from Theorem (3-5)

$$\omega_{opt} = \frac{2}{1 + \sqrt{1 - \rho^2}} \quad (5-4)$$

The new spectra after the SOR modification is

$$\rho' = \begin{cases} (\omega_{opt} - 1) & \omega > \omega_{opt} \\ \left[ \frac{\omega_{opt} \rho_0 + (\omega_{opt}^2 \rho_0^2 - 4(\omega_{opt} - 1))^{1/2}}{2} \right]^2 & \omega < \omega_{opt} \end{cases}$$

Figure 13 shows the effect of a changing  $\omega$  on  $\rho'$  (5-5)

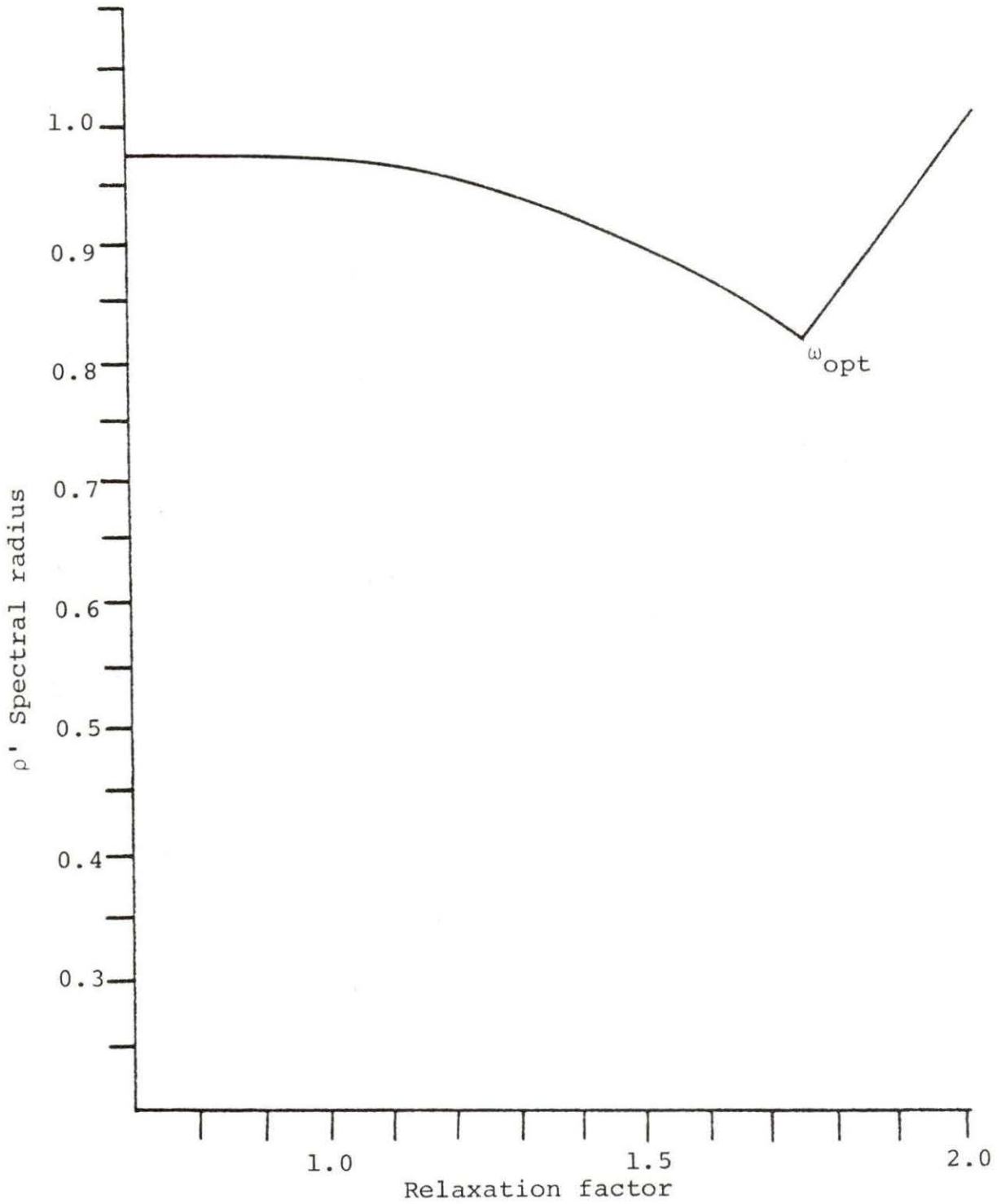


Figure 13.  $\rho'$  vs.  $\omega$  for  $\rho_0 = \cos(\frac{\pi}{20})$

It shows a larger loss of convergence rate will occur if the  $\omega$  is slightly below the optimal value when compared to the case when  $\omega$  is slightly beyond the  $\omega_{opt}$ . This means, if the exact  $\omega_{opt}$  can't be determined, then it is better to overestimate  $\omega$  instead of underestimating it.

From Eq. (5-5), if we know  $\rho$  then  $\omega_{opt}$  can be calculated very easily. The traditional way to calculate  $\rho$  is very tedious and time consuming (it may take more computing time than the direct solutions). There are two strategies to estimate  $\omega$  depending upon what the problem is. If a series calculation based on the same reactor is to be performed, then we can try several different  $\omega$ 's and a curve like Fig. 13 can be plotted. The optimal  $\omega$  can be determined from the curve. This  $\omega_{opt}$  can be used in the succeeding calculations. If the reactor problem is different every time, then a different approach would be applied. The calculation would start with a nonoptimal  $\omega$ , then while the calculation is proceeding, a new  $\rho$  is continually estimated. Theoretically, if the estimating formula is suitable, the estimated  $\rho$  will approach the exact  $\rho$  and the optimal  $\omega$  then can be found. The practical problem is that the time spent in the calculation for finding the  $\omega_{opt}$  should not exceed, say, some certain percentage of the computing time when no relaxation technique is used.

In this research, both strategies are applied and the

results are compared.

## 2. SOR with a fixed relaxation factor

The easiest way to use the SOR method is to apply a fixed-value relaxation factor, because there is no need to calculate  $\rho$  for the determination of the optimal relaxation factor. On the other hand, the convergence will not be the fastest.

Table 2 shows the comparison of the convergence rate between a nonaccelerated calculation (data with \* mark) and an accelerated calculation. The relaxation factors used in the accelerated calculation are chosen arbitrarily; all are 0.5. The convergence rate is not very satisfactory, but it is much better than the nonaccelerated calculation which did not converge.

If all the calculations are based on the same reactor then we may try to find the optimal relaxation factors by going through a thorough search. Since we have four relaxation factors waiting to be optimized and possibly there are interactions between these relaxation factors, an iterative-like approach will be used to find the optimal combination of the relaxation factors.

The process starts by keeping three factors at one fixed value and by changing the value of the remaining one. An optimal value for this relaxation factor can be observed

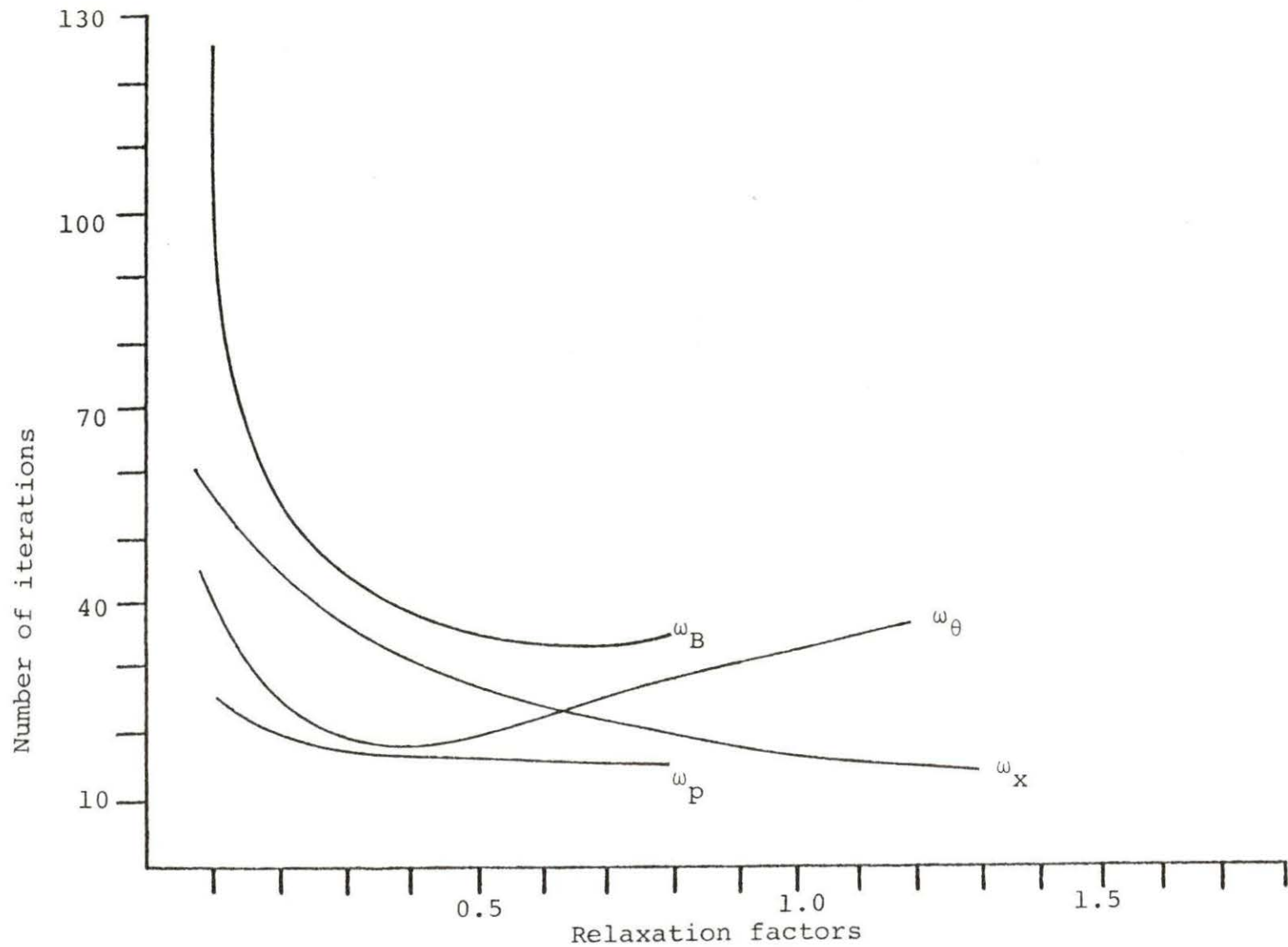


Figure 14. Find the optimum set of relaxation factor



under such circumstances. Using the same procedure, one can find the optimal values for the other three factors. After the optimal values are obtained, the same procedure can be tried again but with a different sequence. If these factors are linearly independent, then the same optimal values should be observed.

Fig. 14 shows the result from the calculation. The optimum combination for the sample problem was 0.7, 1.1, 0.4 and 1.3 for buckling, partial flux, interface average flux and assembly average flux relaxation factors.

### 3. SOR with varying relaxation factor

The exact eigenvalue is difficult to find before the iteration starts, but we may try to estimate it while the iteration process is going. The estimation mechanism is based upon the following explanation [3].

If  $A$  is the iteration matrix and there are  $n$  elements within  $A$ , there are also  $n$  eigenvalues  $\rho_i$ ,  $i=1, n$ , corresponding to each element. These eigenvalues are the sources of the error in the sense of the difference between the exact solution and current estimated value at iteration  $\ell$ .

$$X_i^{(\infty)} - X_i^{(\ell)} = \sum_j A_{ij} \rho_j^{(\ell)} \quad (5-6)$$

As  $\ell \rightarrow \infty$ ,  $\rho_j^\ell \rightarrow 0$  (because  $\rho_j < 1$ ), the contribution from the largest  $\rho_j$  will dominate the error decay rate. Elimination

of the constant  $A_{i,j}$  from Eq. (5-6) results in

$$\frac{X_i^{(\infty)} - X_i^{(\ell)}}{X_i^{(\infty)} - X_i^{(\ell-1)}} \approx \rho \approx \frac{X_i^{(\ell)} - X_i^{(\ell-1)}}{X_i^{(\ell-1)} - X_i^{(\ell-2)}} \quad (5-7a)$$

and

$$\frac{X_i^{(\infty)} - X_i^{(\ell)}}{X_i^{(\ell)} - X_i^{(\ell-1)}} \approx \frac{\rho}{1.0-\rho} \quad (5-7b)$$

The absolute error is reduced by  $\rho$  after each iteration and the ratio between the absolute error  $(X_i^{(\infty)} - X_i^{(\rho)})$  to the iterate change depends upon the reciprocal of  $1.0-\rho$ . These two formulas give a practical and efficient way to estimate the eigenvalue which in turn can be used to find the optimal relaxation factor. The estimating formula (5-7) can be used to find the ratio between two succeeding absolute errors; the ratio will approach the eigenvalue. The estimation can be started after several iterations have been performed. This will reduce the fluctuations. Also, the estimating calculation doesn't need to be performed at every iteration because the approach to the eigenvalue is quite smooth. Based upon investigation of the iteration behavior, the appropriate time to estimate  $\rho$  can be decided. However, in this research, the estimation was performed every 8 iterations. Fig. 15 shows that  $\rho$  approaches a constant as the number of iterations increases.

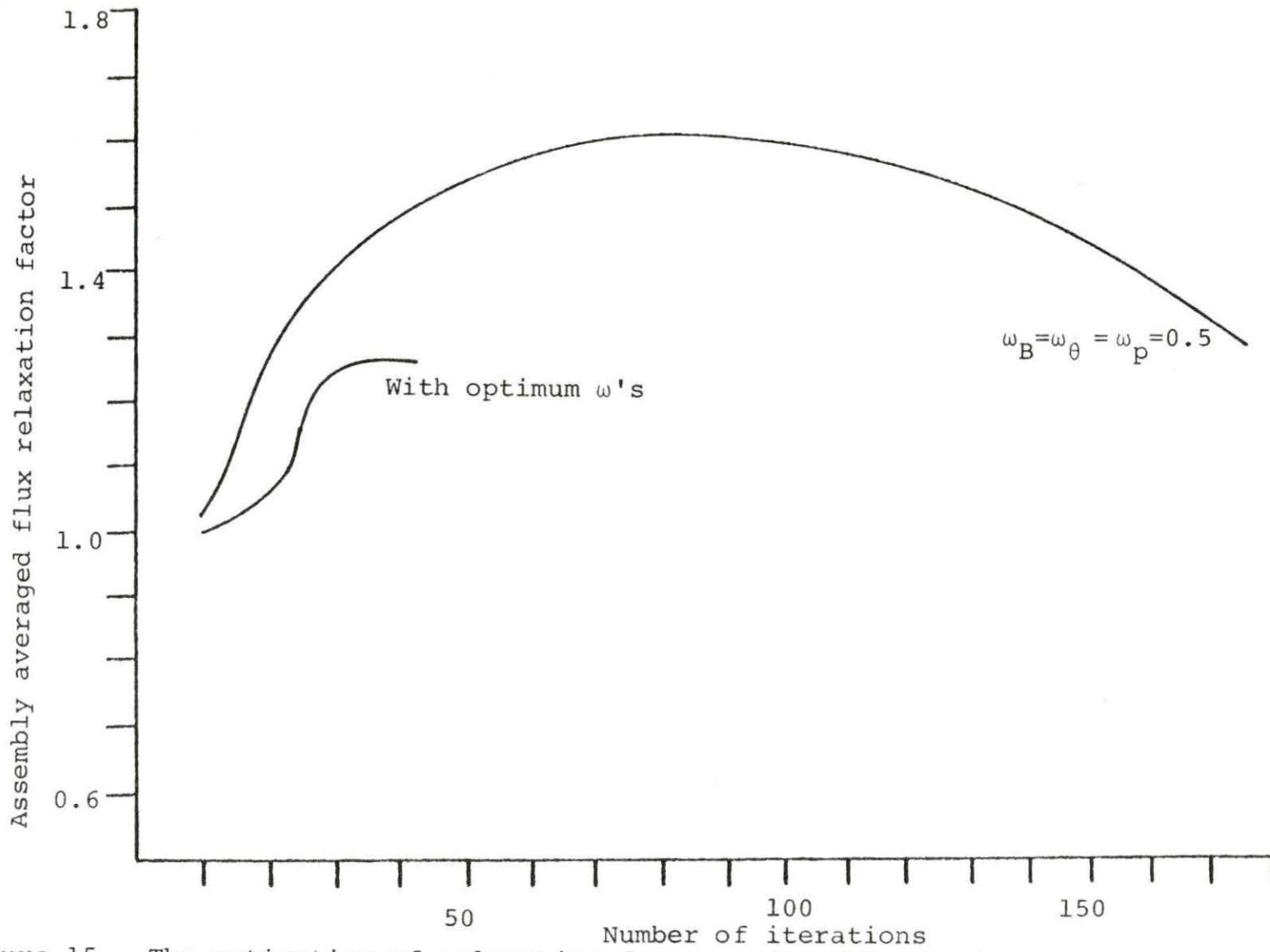


Figure 15. The estimation of relaxation factor under SOR method

Fig. 16 and Fig. 17 shows the error decay behavior.

Table 2 gives the idea of the effectiveness of the acceleration technique.

Table 2. The effectiveness of SOR

$\epsilon$	Number of iterations to reduce error to $\epsilon$		
	Without acceleration <sup>a</sup>	SOR with $\omega_B = \omega_p = \omega_\theta = 0.5$	SOR with optimum $\omega$ 's
0.01	16	16	10
0.001	50	50	19
0.0001	185	97	30
0.00001	>300	145	41
0.000001	>300	194	48

<sup>a</sup> Does not converge.

### C. Application of Nonstationary Accelerating Techniques [12]

The general form for a nonstationary method is

$$U^{(\ell+1)} = G^{(\ell)} U^0 + k'_\ell$$

where

$$G^{(\ell)} = G_\ell G_{\ell-1} \dots G_0$$

and

$$k'_\ell = k_\ell + G_{\ell-1} k_{\ell-1} + \dots + G_2 k_1$$

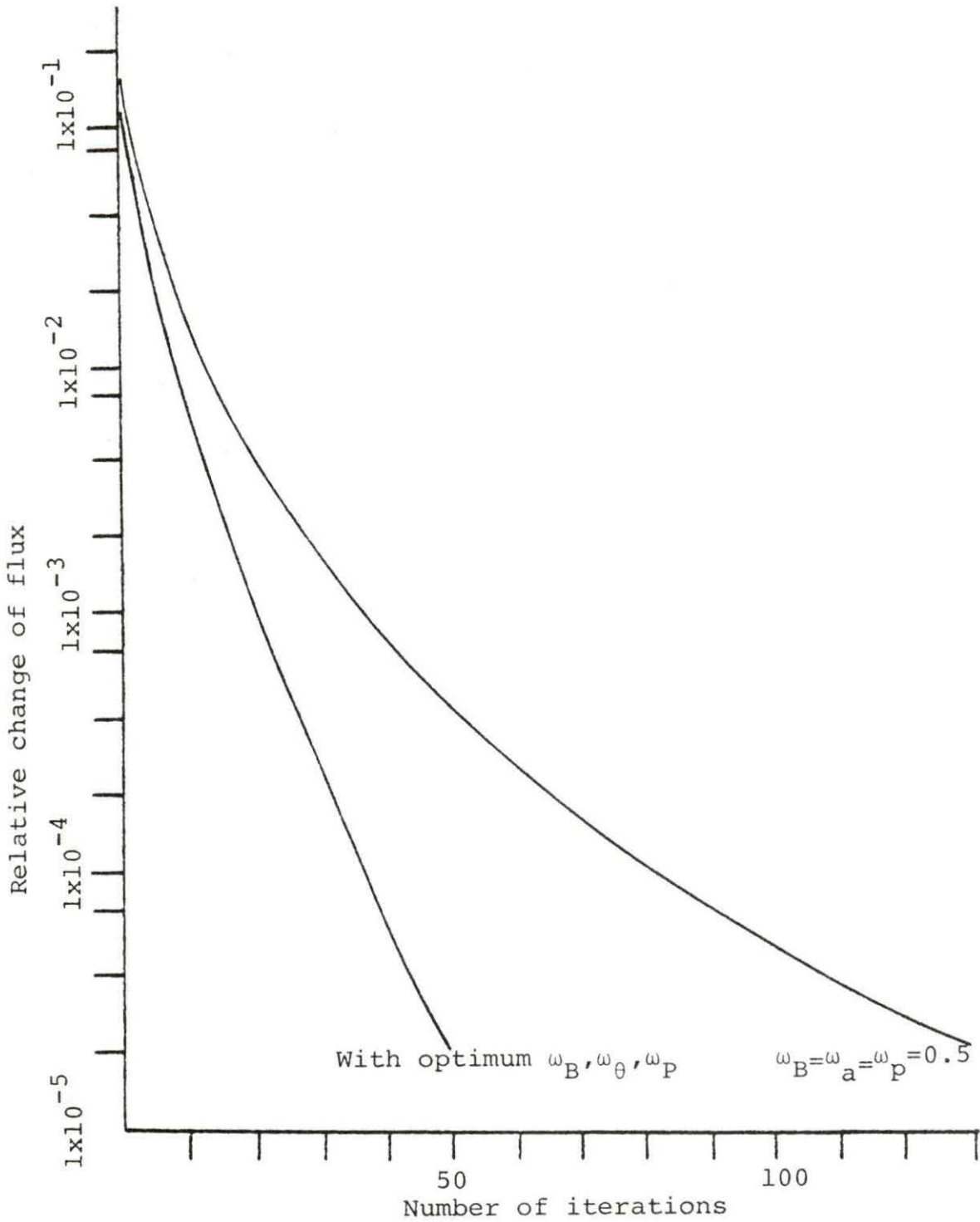


Figure 16. Error decay behavior under SOR method

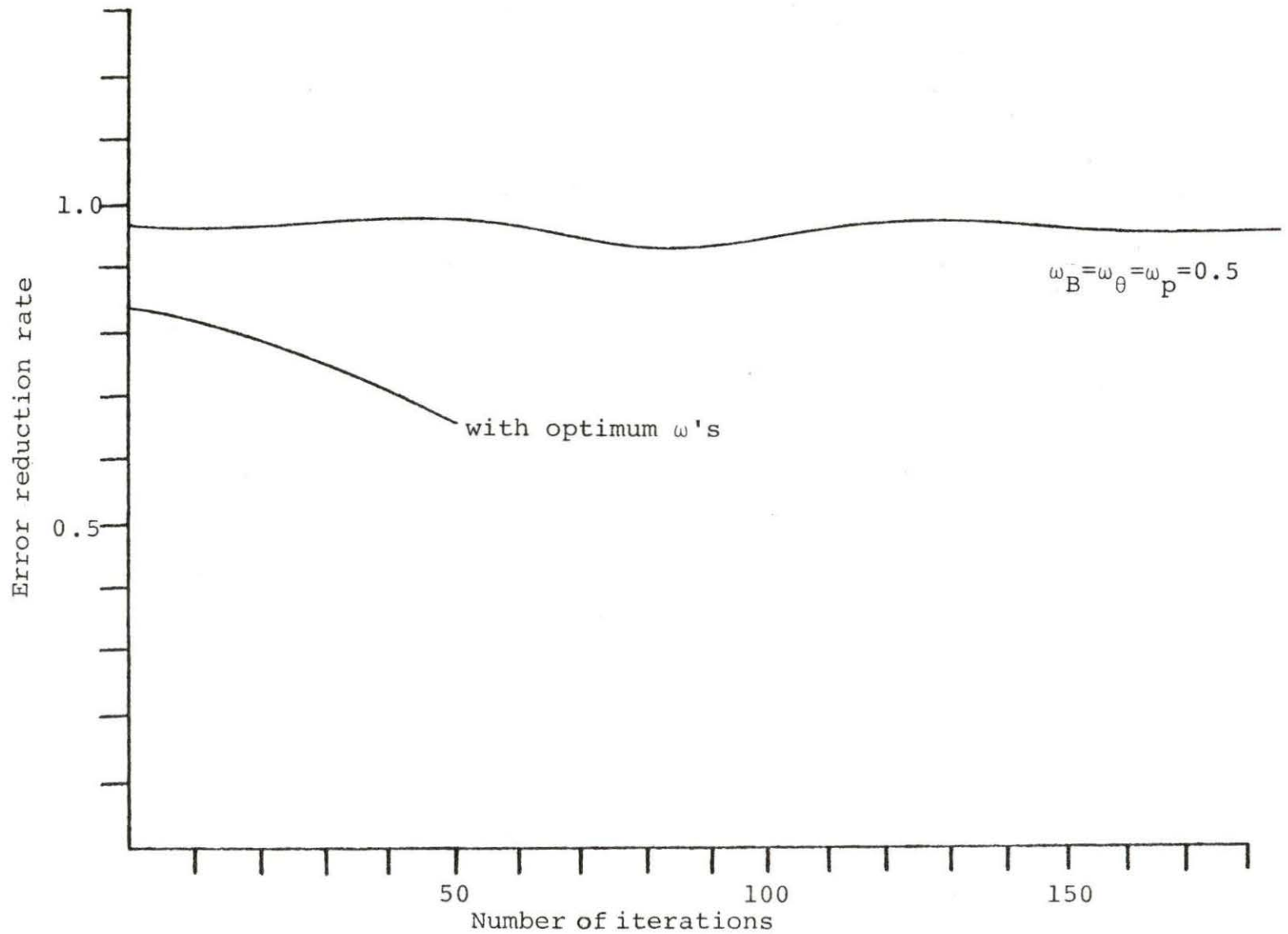


Figure 17. Error reduction rate under SOR method

Given a stationary iterative method, one can often find an associated nonstationary method which will converge faster than the given method. In the following paragraphs, a nonstationary method will be derived based on the SOR method which was introduced earlier in this chapter.

### 1. The minimax problem

The derivation starts with a general form of the SOR method

$$\phi^{(t+1)} = [1 + \theta^{(t)}] \phi^* - \theta^{(t)} \phi^{(t)} \quad (5-8)$$

where the relation to the  $\omega$  in Eq. (5-4) is

$$\omega = 1 + \theta$$

Consider the matrix form of the iteration formula

$$A\phi^{(t)} = \lambda^{(t)} \phi^{*(t+1)} \quad (5-9)$$

Combine (5-8) and (5-9)

$$\phi^{(t+1)} = [(1+\theta^{(t)}) \frac{A}{\lambda^{(t)}} - \theta^{(t)} I] \phi^{(t)} \quad (5-10)$$

Define R as  $R_t = [\frac{1+\theta^{(t)}}{\lambda^{(t)}}]A - \theta^{(t)} I$

Then (5-10) can be rewritten as

$$\phi^{(t+1)} = R_t \phi^{(t)} \quad (5-11)$$

then it is obvious

$$\phi^{(t+1)} = R_n R_{n-1} \dots R_1 R_0 \phi^{(0)} \quad (5-12)$$

Assume there are  $m$  eigenvalues and  $m$  eigenvectors of  $A$  represented by

$$\sigma_m < \sigma_{m-1} < \dots < \sigma_1, \quad (5-13)$$

$$\alpha_m, \alpha_{m-1}, \dots, \alpha_1$$

these eigenvectors form a complete set for the vector space of  $H$ .

The initial guess can be represented in terms of these eigenvectors

$$\phi^{(0)} = \sum_{k=1}^m C_k \alpha_k \quad (5-14)$$

Since  $\alpha_k$  is an eigenvector of  $A$ , then we can write

$$\begin{aligned} R_j \alpha_k &= \left[ \frac{1+\theta^{(i)}}{\lambda^j} \right] A \alpha_k - \theta^{(j)} \alpha_k \\ &= \left[ \frac{1+\theta^{(j)}}{\lambda^{(j)}} \sigma_k^{-\theta^{(j)}} \right] \alpha_k \end{aligned} \quad (5-15)$$

Plugging (5-14) into (5-15), we find

$$\phi^{(\ell)} = \prod_{j=0}^{\ell-1} R_j \sum_{k=1}^m C_k \alpha_k$$

or

$$\phi^{(\ell)} = \sum_{k=1}^m C_k \prod_{j=0}^{\ell-1} \left[ \frac{1+\theta^{(j)}}{\lambda^{(j)}} \sigma_k^{-\theta^{(j)}} \right] \alpha_k \quad (5-16)$$

Because the convergence rate is dominated by the largest



eigenvalue  $\sigma_1$  and its associated eigenvector  $\alpha_1$ , Eq.

(5-16) can be rewritten as

$$\phi^{(\ell)} = \prod_{j=0}^{\ell-1} \left[ \frac{1+\theta^j}{\lambda^j} \sigma_1^{-\theta^j} \right] \left\{ C_1 \alpha_1 + \sum_{k=2}^m \left[ \frac{\sigma_k - \frac{\lambda^j \theta^j}{1+\theta^j}}{1 - \frac{\lambda^j \theta^j}{1+\theta^j}} \right] \alpha_k \right\} \quad (5-17)$$

or

$$\phi^{(\ell)} = f_\ell \left[ C_1 \alpha_1 + \sum_{k=2}^m C_k g_\ell(\theta, \sigma_k) \alpha_k \right] \quad (5-18)$$

where

$$f_\ell = \prod_{j=1}^{\ell-1} \left[ \frac{1+\theta^j}{\lambda^j} \sigma_1^{-\theta^j} \right] \quad (5-19)$$

and

$$g_\ell = \prod_{j=0}^{\ell-1} \left[ \frac{\sigma_k - \frac{\lambda^j \theta^j}{1+\theta^j}}{1 - \frac{\lambda^j \theta^j}{1+\theta^j}} \right] \quad (5-20)$$

From Eq. (5-18) we can find the criterion for choosing the optimum set of extrapolation parameters  $\theta^j$  such that the function  $g_\ell(\theta, \sigma_k)$  will have a minimum value.

By changing variable

$$\mu = \frac{2\sigma}{\sigma_2^{-\sigma_m}} - \frac{\sigma_2^{+\sigma_m}}{\sigma_2^{-\sigma_m}} \quad (5-21)$$

then

$$h_\ell(\theta, \mu) = g_\ell(\theta, \sigma)$$

Now we seek the polynomial which minimizes

$$\max_{-1 \leq \mu \leq 1} |h_\ell(\theta, \mu)|$$

This is a typical minimax problem often found in approximation problems.

## 2. Chebyshev polynomials

From the study of approximation problems and the characteristics of Chebyshev polynomials, the following theorem gives the solution to this minimax problem.

Theorem 5-1: [13] Among all polynomials of degree  $m$  in  $\mu$  having the value  $+1$  at  $\mu_1 > 1$ , there is just one having the minimum-maximum absolute value throughout the interval  $(-1, +1)$ , namely the polynomial.

$$S_m(\mu) = T_m(\mu) / T_m(\mu_1) \quad (5-22)$$

where  $T_m(\mu)$  is the  $m^{\text{th}}$ -order Chebyshev polynomial, obtained by expanding

$$T_m(\mu) = \cos(m \cos^{-1} \mu) \quad (5-23)$$

in powers of  $\mu$ .

To make

$$h_n(\theta, \mu) = \frac{T_n(\mu)}{T_n(\mu_1)}$$

we can equate the zeroes of each polynomial since they both

have the same value at  $\mu = \mu_1$ .

The zeroes for  $T_n(\mu)$  are

$$\mu_\ell = \cos \frac{(2\ell+1)\pi}{2n}, \quad \ell=0, \dots, n-1 \quad (5-24)$$

The zeroes for  $h_n(\theta, \mu)$  are

$$\mu_\ell = \frac{2}{\sigma_2 - \sigma_m} \left[ \frac{\lambda^\ell \theta^\ell}{1 + \theta^\ell} \right] - \frac{\sigma_2 + \sigma_m}{\sigma_2 - \sigma_m}, \quad \ell=0, 1, \dots, n-1. \quad (5-25)$$

Equating Eqs. (5-24) and (5-25), one has

$$\theta^{(\ell)}(n) = \frac{1 + \left( \frac{\sigma_2 - \sigma_m}{\sigma_2 + \sigma_m} \right) \cos \frac{(2\ell+1)\pi}{2n}}{\frac{2\lambda^{(\ell)}}{(\sigma_2 + \sigma_m)} - 1 - \left( \frac{\sigma_2 - \sigma_m}{\sigma_2 + \sigma_m} \right) \cos \frac{(2\ell+1)\pi}{2n}} \quad (5-26)$$

This is the optimal set of relaxation factors which will give the best result.

### 3. The implementation

To apply the result given by Eq. (5-26), the eigenvalues  $\sigma_2$  and  $\sigma_m$  must be known in advance; this turns out to be the same problem which happened in the stationary SOR method because we are never privileged to have eigenvalues on hand in a practical case. Some more approximations must be made before we can put this theory into practice.

To reduce Eq. (5-26) to a simpler form, the  $\sigma_m$  may be neglected by comparison to  $\sigma_2$ , then we get

$$\theta^{(\ell)}(n) = \frac{1 + \cos\left[\frac{(2\ell+1)\pi}{2n}\right]}{\frac{2\lambda^{(\ell)}}{\sigma_2} - 1 - \cos\left[\frac{(2\ell+1)\pi}{2n}\right]} \quad (5-27)$$

Now, define

$$\bar{\sigma} = \max_{i \neq 1} \left| \frac{\sigma_i}{\sigma_1} \right| = \frac{\sigma_2}{\sigma_1}$$

and

$$C_\ell(n) = 1 + \cos \frac{2\ell+1}{2n}\pi$$

therefore, (5-27) becomes

$$\theta^{(\ell)}(n) = \frac{\bar{\sigma} C_\ell(n)}{2 - \bar{\sigma} C_\ell(n)} \quad (5-28)$$

The parameter  $\bar{\sigma}$  is often called the dominance ratio. Since it gives the magnitude of the separation between the largest eigenvalue and the second largest.  $\bar{\sigma}$  is estimated by

$$\bar{\sigma} = \frac{R^{(\ell)}}{R^{(\ell-1)}} \quad (5-29)$$

where

$$R^{(\ell)} = \sum_{i=1}^{\pi} (\phi_i^{(\ell)} - \phi_i^{(\ell-1)})$$

Now we need to determine what degree Chebyshev polynomial will be likely to reduce the eigenvalue error to an acceptable value. The maximum value of  $|h_n(\mu)|$  in interval  $[-1, 1]$  is  $1/T_n(\mu_1)$ . This can be taken as a measure of the reduction of the coefficients of all eigenvectors with

eigenvalue in the range  $\sigma_m$  to  $\sigma_2$ .

Since

$$\mu_1 = \mu(\sigma_1) = \frac{2\sigma_1}{\sigma_2 - \sigma_m} - \frac{\sigma_2 + \sigma_m}{\sigma_2 - \sigma_m},$$

neglect  $\sigma_m$ ,

$$\mu_1 \approx \frac{2\sigma_1}{\sigma_2} - 1 = \frac{2}{\sigma} - 1$$

Define

$$\varepsilon(\ell) = \frac{\lambda^{(\ell)} \underline{\lambda}^{(\ell)}}{\lambda^{(\ell)}} \quad (5-30)$$

Assume  $\varepsilon_1$  is a preset criterion, then the degree of Chebyshev polynomial is decided such that

$$\frac{\varepsilon^{(\ell)}}{T_n\left(\frac{2}{\sigma} - 1\right)} < \varepsilon_1. \quad (5-31)$$

We perform a cycle of iterations using a sequence of  $\theta$ 's given by Eq. (5-28),  $\ell=0,1,\dots,n-1$ . If convergence still has not been achieved, a new  $n$  is calculated based on the inequality (5-31) and another cycle of  $n$  iterations is performed.

Fig. 18 shows the error reduction relative to the number of iterations, Fig. 19 shows the convergence rate vs. number of iteration.

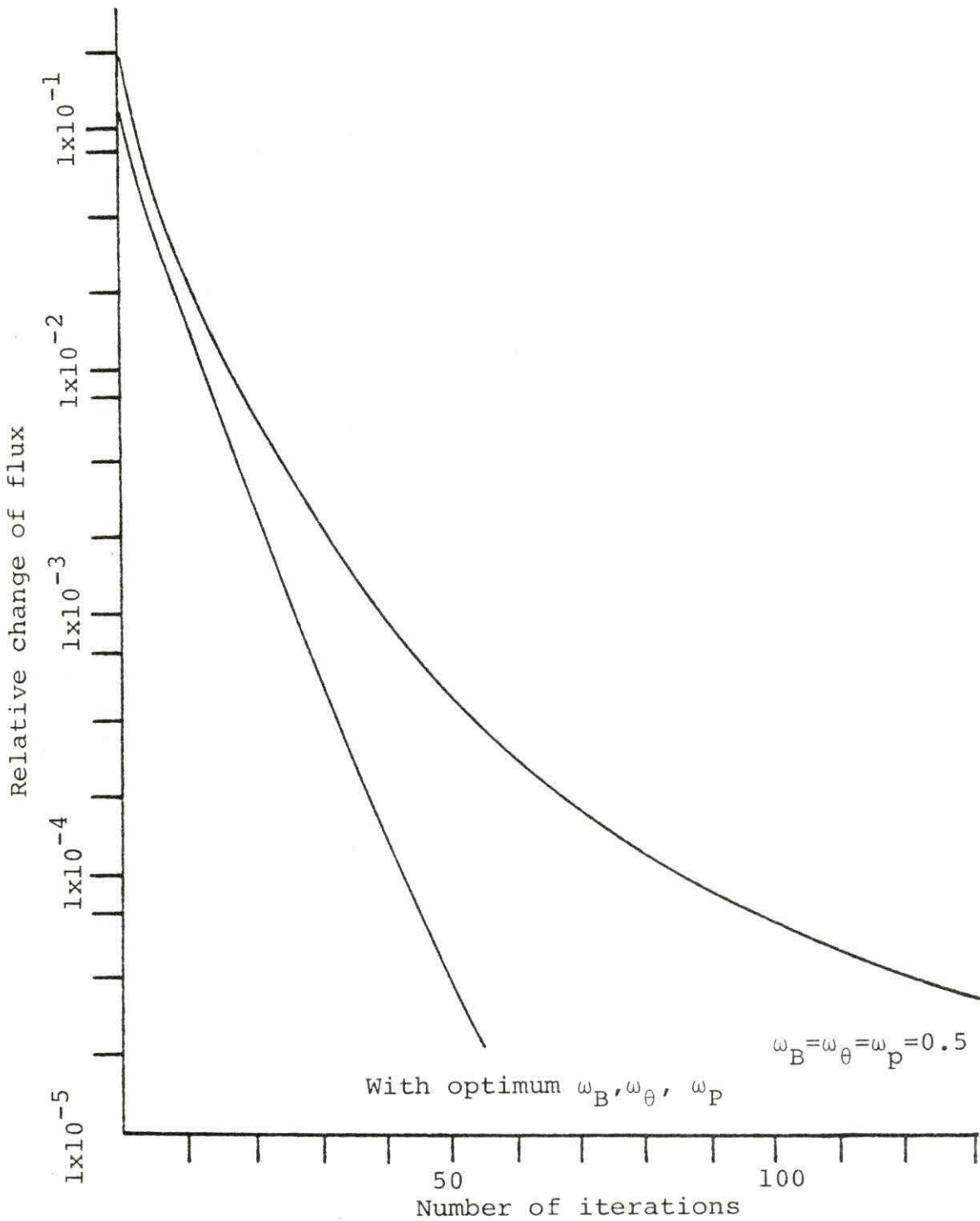


Figure 18. Error decay behavior under Chebyshev extrapolation

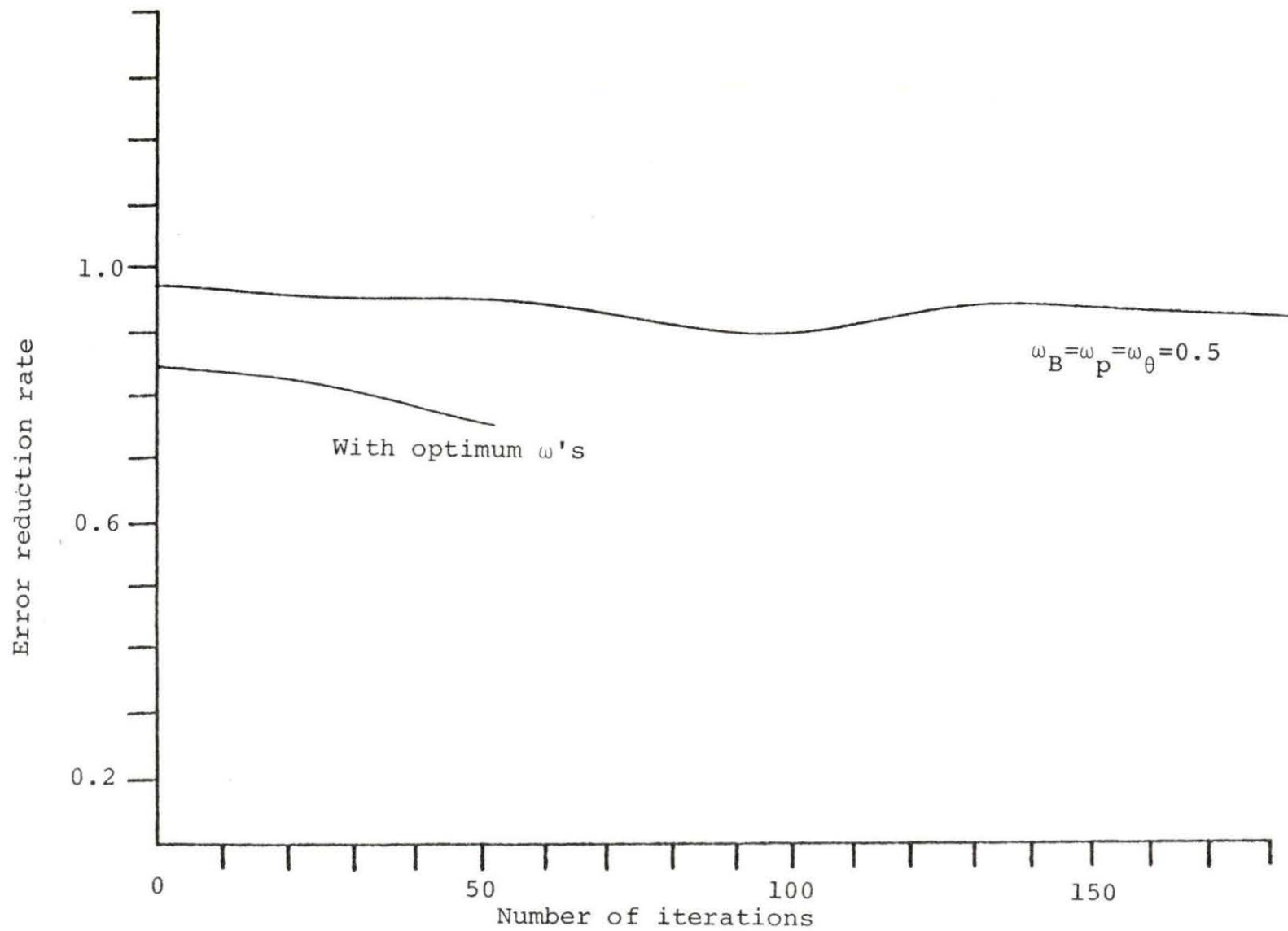


Figure 19. Error reduction rate under Chebyshev extrapolation

## C. Comparison of Methods

Table 3 shows the results of a nonaccelerated calculation, the iteration process is very unstable and diverges. Table 4 shows the comparison between these two acceleration methods in terms of the number of iterations needed to reduce the error down to a specific criterion. Case 1, acceleration with optimal relaxation factors, has the best result and is almost 10 times faster than the case 2 in which all relaxation factors were chosen arbitrarily. Case 3 is SOR with a varying relaxation factor. The convergence rate is twice that of case 2, but it is slower than case 1.

The Chebyshev calculation behaves very much like the SOR method. Theoretically, the Chebyshev extrapolation should have faster rate than the SOR method. The reason this does not happen is because the estimation of some of the key terms is not accurate enough. This reduces the effectiveness of the Chebyshev extrapolation.

If accelerating techniques are applied with  $\omega_B$ ,  $\omega_\theta$ ,  $\omega_p$  all at their optimal values, an improvement by 3-4 times faster is observed. This accounts for the interactive influence between these relaxation factors.



Table 3. Calculation without acceleration

Iterations	$\max_{i=1}^n \phi_i^{(\ell)} - \phi_i^{(\ell-1)}$	$[\sum_{i=1}^n (\frac{\phi_i^{(\ell)}}{\phi_i^{(\ell-1)}} - 1)^2]^{1/2}$
1	0.230	0.0841
2	0.184	0.0804
3	0.215	0.0867
4	0.281	0.1159
5	0.440	0.1587
6	0.641	0.24134
7	0.968	0.4097
8	4.191	2.66481
9	2.351	3.09604
10	995.918	414.128

Table 4. Comparison between different accelerating techniques

	Number of iterations needed to reduce the relative error to:				
	0.01	0.001	0.0001	0.00001	0.000001
1. SOR with optimal factors	6	12	19	28	39
2. SOR with arbitrary chosen factors <sup>a</sup>	9	33	133	267	X
3. SOR with variable relaxation <sup>b</sup>	11	32	78	131	194
4. SOR with variable relaxation <sup>c</sup>	11	26	37	42	48
5. Chebyshev <sup>d</sup>	10	29	81	128	207
6. Chebyshev <sup>e</sup>	8	22	35	53	55

<sup>a</sup>  $\omega_B = \omega_P = \omega_\theta = \omega_X = 0.5$ .

<sup>b</sup>  $\omega_B = \omega_P = \omega_\theta = 0.5$ ,  $\omega_X$  is calculated by (5-4).

<sup>c</sup>  $\omega_B = 0.7$ ,  $\omega_P = 1.1$ ,  $\omega_\theta = 0.4$ ,  $\omega_X$  is calculated by (5-4).

<sup>d</sup>  $\omega_B = \omega_P = \omega_\theta = 0.5$ ,  $\omega_X$  is calculated by (5-28).

<sup>e</sup>  $\omega_B = 0.7$ ,  $\omega_P = 1.1$ ,  $\omega_\theta = 0.4$ ,  $\omega_X$  is calculated by (5-28).

## VI. SUMMARY AND CONCLUSIONS

The complete theory of acceleration mechanisms has not been fully developed [ 3], and many acceleration techniques are only based upon experience and empirical formulas [14, 15]. Although in some cases the optimal accelerating parameter can be formulated (4-16 and 4-17), the actual evaluation of the formulas may take prohibitive computational times. An approximation is always needed which is a deficiency of the technique. However, the overall performance is improved, sometimes impressively, as we saw in earlier discussions.

Besides the SOR and Chebyshev extrapolation accelerating techniques, there are other different techniques being used widely, e.g., the ADI method, the conjugate gradients method, etc. The reason we didn't try these methods is that they are much more matrix-oriented techniques, i.e., a complicated matrix representation and manipulation are required when applying the technique. This turns out to be the current major concern of the Neutron Diffusion-Nodal model--the matrix form of this model which has not been developed completely. Although this model behaves quite well in many aspects, a strict and complete matrix representation will be very important if further improvement is expected.

There are four relaxation factors which are adjustable

and need to be optimized. There is a strong interactive influence among these factors. A closer study of the interrelation of these factors may lead to the simplification of the whole model. The reason is that if some of the relaxation factors could be combined into one single factor, then both the computational procedure and acceleration process might be simplified significantly.

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