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Formulation and analysis of higher order finite difference approximations to the neutron diffusion equation

Mohammed Benganem
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FORMULATION AND ANALYSIS OF HIGHER ORDER FINITE DIFFERENCE
APPROXIMATIONS TO THE NEUTRON DIFFUSION EQUATION

Iowa State University

PH.D. 1986

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Formulation and analysis of higher order finite difference
approximations to the neutron diffusion equation

by

Mohammed Benghanem

A Dissertation Submitted to the
Graduate Faculty in Partial Fulfillment of the
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1986

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NOMENCLATURE

A.D.I.	Alternating direction implicit method
ANAL	Analytical solution
F.D	Finite difference
F.D.E	Finite difference equation
H_x or H_1	Step size in x direction
H_y or H_2	Step size in y direction
H_z or H_3	Step size in z direction
PDE	Partial differential equation
RHS	Right hand side
S.D.	Significant digits
T.E	Truncation error
VAST	Vector and array syntax translator
2-D	Two dimensions
3-D	Three dimensions
ϕ_{ijk}	Numerical approximation to the function $\phi(x,y,z)$ at node (i,j,k)
$\phi(x_i, y_j, z_k)$	Exact value of $\phi(x,y,z)$ at point (x_i, y_j, z_k)
ϕ_o or	
$\phi(x_o, y_o, z_o)$	Numerical approximation of the function ϕ at the central node (i,j,k)

I. INTRODUCTION AND LITERATURE REVIEW

I.1. Preamble

Many of the partial differential equations from engineering and scientific applications can only be solved numerically. Finite difference approximations have been one of the most used techniques. Since the forties, due to rapid advances in computer technology, these numerical schemes have become very popular [1]. Thus, in nuclear engineering, several famous codes were developed using finite difference techniques [2-5].

Currently, in the published literature, the nuclear reactor calculational trends have shifted toward nodal and coarse mesh methods as reviewed in the paper of Dorning [6]. In spite of their considerable theoretical potential, these new methods have had only limited practical use [6, 7], especially for detailed three-dimensional problems. Therefore, in cases such as the design of a new fuel assembly or in reactor safety analysis, where details and high accuracy are required, researchers still use computer codes established upon finite difference techniques [7, 8]. Reference [9] contains abstracts of some of these programs, including DIF3D [10] and a recent version of PDQ called PDQ-8 [11].

Furthermore, when using finite difference techniques (or any other numerical scheme), analysts are mainly concerned with:

- a. Computer memory
- b. Speed of computation.

Even though three-dimensional (3-D) problems are of great practicality,

hitherto they have not reached the maturity expected due to their ineffectiveness toward the above concerns [12].

In spite of the foregoing, the objective of this research will be to undertake the formulation and analysis of a 3-D finite difference approximation, motivated by the following:

1. The need to extend the schemes developed by Eckholtz [13], Al-Dujaili [14] and Kadri [15].
2. The possibility to incorporate the 27-point relations into the existing 7-point codes [16].
3. The attempt to show that finite difference can be practically feasible, without causing computational detriment of an improved higher order formulation.
4. The improvement in the numerical methods can be of great importance because, as Henry stated in an international meeting on numerical reactor calculation [17]:

Theoretical people are not terribly expensive compared with, say a pressure vessel or with the cost implications involved in a tenth-of-a-percent change in fuel enrichment. In fact, we are pretty cheap in comparison, and it seems to me that to stop that sort of analytical development is not good long-range planning.

5. Another stimulus to this investigation is the advent of the supercomputer which vectorizes numerical calculations so as to make calculations several magnitudes faster than using the usual systems [9, 18]. The vector processor might be used to enhance the speed of computation.
6. Finally, the overall aspect of this project will be to

develop finite differences recipes for the reactor equations which can be readily used for other equations which are based upon the Laplacian operator.

I.2. Literature Review

The basis of this study is the model developed by Rohach [19]. This higher order F-D approximation is similar to that of Greenspan [20] in the case of nonequal spacings and to that of Bickley [21] and others [22-25] if the equal spacings in both directions are considered.

H. Van Linde [26] achieved a 4th order F-D approximation for the Poisson's equation in 2-D. He demonstrated that his results are more efficient than the ones obtained by Bramble et al. [27]. Furthermore, Bramble [28] extended his procedure to the 3-D Dirichlet problem for Poisson's equation. In addition to being of 4th-order accuracy, the scheme was constrained to the case where both the unknown function (U) and the RHS function (F) should be sufficiently smooth. Another important approximation was established by Rosser [29]. He constructed a 6th order finite difference approximation for Poisson's equation in 2-D. His method has the same restrictions mentioned above. Moreover, some of his coefficients were negative. This fact might cause problems as was pointed out in the report by Lynch [30]. Lynch also developed an $O(h^6)$ finite difference approximation to the Helmholtz equation in n-D [31]. He said, "One cannot obtain an $O(h^6)$ approximation by using only 27 lattice points used for the operator L_h " (L_h is the discrete representation of ∇^2). He also pinpointed some disadvantages of his

scheme. His method, called HODIE [32], was modified and implanted in the famous ELLPACK Code [33].

The essential differences between the present model and the above approaches are:

1. Improved truncation error without the restrictions to square meshes, as was demonstrated by Eckholtz and Kadri.
2. No prior assumptions either on the unknowns or on the RHS function F (except the conditions implied by the use of the Taylor's expansion; i.e., analyticity of the functions [34]).
3. No negative coefficients; therefore, no subsequent problems with reducing round-off error [30].

As usual, the application of finite difference results in a system of equations which might be linear or nonlinear. In three dimensions, this system can be very large. To solve it, two general strategies exist. These are the direct (or non-iterative) and the iterative methods [35]. The former method has had only limited progress in three dimensions [36, 37] except for separable elliptic problems where they have proven to be very effective [38]. In contrast, iterative techniques, even with their shortcomings regarding the round-off error [39, 40], have widespread use, especially for large systems. Moreover, these methods may be categorized as stationary and non-stationary. The SOR (successive overrelaxation) method [35], with its various options (point, line, block relaxation, symmetric, etc.), the Gradient Conjugate method and the ADI (alternative direction implicit) method [41] are the most popular.

Even though the author is aware that other techniques [42, 43] could be applied efficiently, because of the ease in programming, the SOR will be used in this study.

II. THEORETICAL DEVELOPMENT

II.1. The Neutron Diffusion Equation

The one-speed neutron diffusion equation in a steady state critical reactor is given [44] by:

$$\underline{\nabla}[D(\underline{r})\underline{\nabla}\phi(\underline{r})] - \Sigma_a(\underline{r})\phi(\underline{r}) + v\Sigma_f\phi(\underline{r}) = 0 \quad (1)$$

where:

$\phi(\underline{r})$ = neutron flux,

$$\underline{\nabla} = \frac{\partial}{\partial x} \hat{i} + \frac{\partial}{\partial y} \hat{j} + \frac{\partial}{\partial z} \hat{k},$$

$D(\underline{r})$ = diffusion coefficient,

$\Sigma_a(\underline{r})$ = absorption cross-section,

$S(\underline{r})$ = neutron source, and

$\underline{r} = \underline{r}(x, y, z)$

If the media is homogeneous, the material parameters are assumed constant, so that equation 1 gives:

$$D\underline{\nabla}^2\phi(\underline{r}) - \Sigma_a\phi(\underline{r}) + v\Sigma_f\phi(\underline{r}) = 0 \quad (2)$$

Dividing the above equation by D, and defining the buckling as

$$B^2 = \frac{v\Sigma_f - \Sigma_a}{D} \quad (3)$$

Then equation 3 becomes:

$$\underline{\nabla}^2\phi(\underline{r}) + B^2\phi(\underline{r}) = 0 \quad (4)$$

which is the known reactor equation [45]. Moreover, equation 4 with the appropriate boundary conditions constitutes an elliptic problem of

the eigenvalue type [46].

In this study, it will be solved for the eigenvalue (B^2) and the eigenfunction (ϕ), using the higher order accurate finite difference approximations.

The major reasons for considering the above simple equation are:

1. The one-speed neutron diffusion equation is an important equation to study in nuclear engineering.
2. The availability of the analytical solution to use as a benchmark to compare with the numerical solution.
3. The manipulations of the F.D.E. will be simpler, since space and energy are separated.
4. The unsteady state one group equation is valid in a number of physical situations. To use the present model, one is required to find an approximation to the time derivative.
5. The extension to n energy groups would be straightforward.

II.2. The Fundamental Relation

To find the solution of equation 4, one will be mainly concerned with the evaluation of the Laplacian operator. In two dimensions, Rohach [19] developed a nine-point approximation to the Laplacian by considering the following fundamental relation (see Fig. 1):

$$\left(\frac{1}{\beta} - p\right)S_{13} + (\beta - p)S_{24} + \frac{p}{2} C_{1234} \quad (4)$$

where:

$$\beta = \frac{h_1}{h_2}$$

$$S_{13} = \phi_1 + \phi_3$$

$$S_{24} = \phi_2 + \phi_4$$

$$C_{1234} = \phi_{12} + \phi_{23} + \phi_{34} + \phi_{41} \text{ (corners)}$$

p = a parameter, by way of which one establishes the order of truncation error (T.E).

For equal spacing ($h_1 = h_2 = h$), relation 4 becomes:

$$(1 - p)(S_{13} + S_{24}) + \frac{p}{2} C_{1234} \quad (5)$$

One can note that equations 4 and 5 were the basis for Eckholtz's [13] and Kadri's [15] theses.

Our primordial concern will then be to establish the 3-D relations corresponding to equation 4 or 5. However, in this study only a uniform spacing ($h_1 = h_2 = h_3 = h$) will be considered. To achieve this, Fig. 2 is of great relevance.

One can already observe that the main difference from the 2-D molecule is the consideration of the three levels of distance from the central point. The first level includes the face points ($\phi_1, \phi_2, \phi_3, \phi_4, \phi_5$ and ϕ_6). These points are used in the normal seven-point formula. The second level includes the twelve edges points ($\phi_{15}, \phi_{53}, \phi_{36}, \phi_{61}, \phi_{12}, \phi_{23}, \phi_{34}, \phi_{41}, \phi_{25}, \phi_{54}, \phi_{46}$ and ϕ_{62}). The third level includes the eight corner points ($\phi_{125}, \phi_{235}, \phi_{345}, \phi_{364}, \phi_{146}, \phi_{162}, \phi_{263}$ and ϕ_{154}).

Moreover, for the three-dimensional case one will have, similar to equation 5, to introduce two parameters, p and p' . The latter parameter

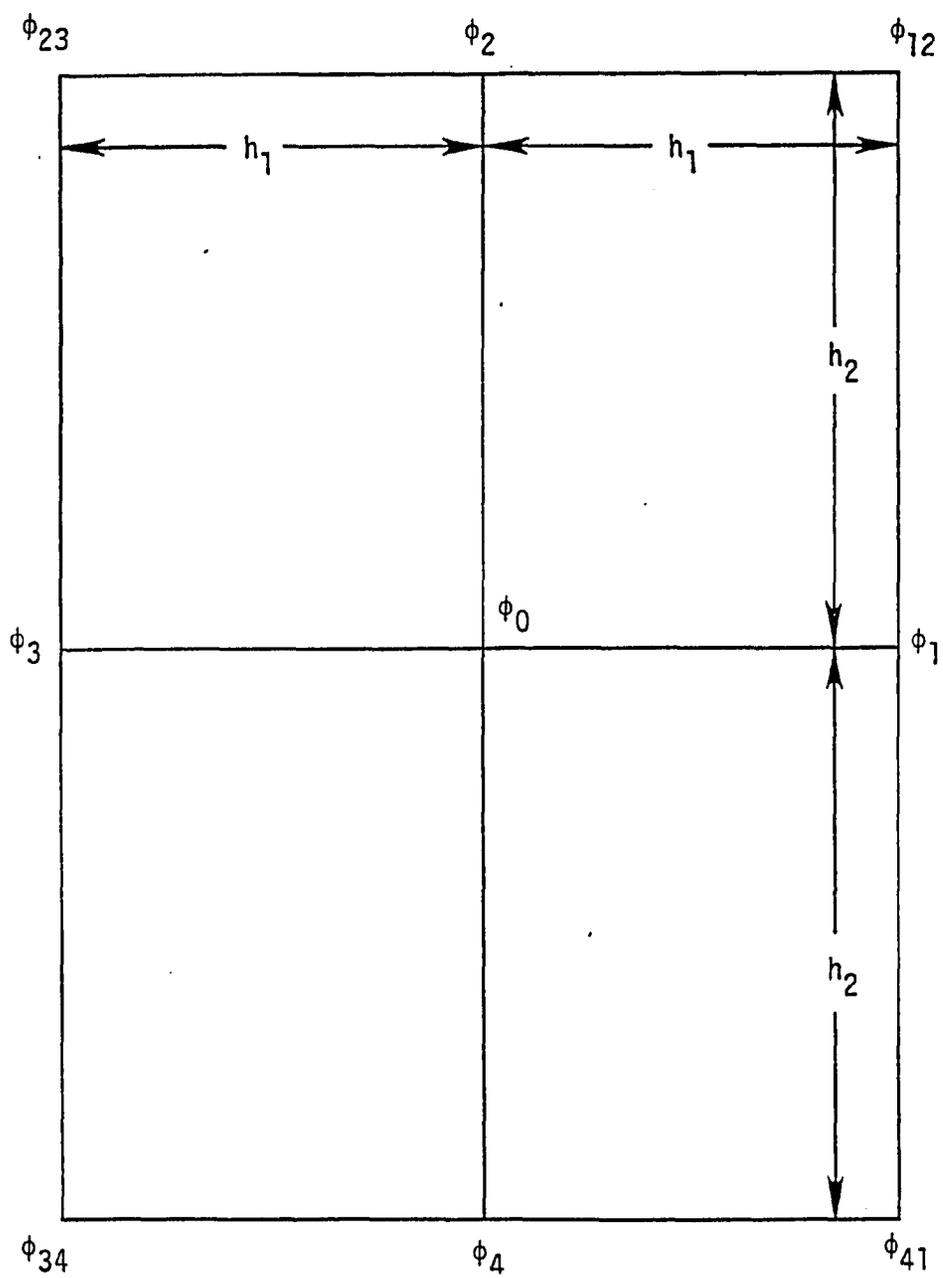


Figure 1. Two-dimensional molecule

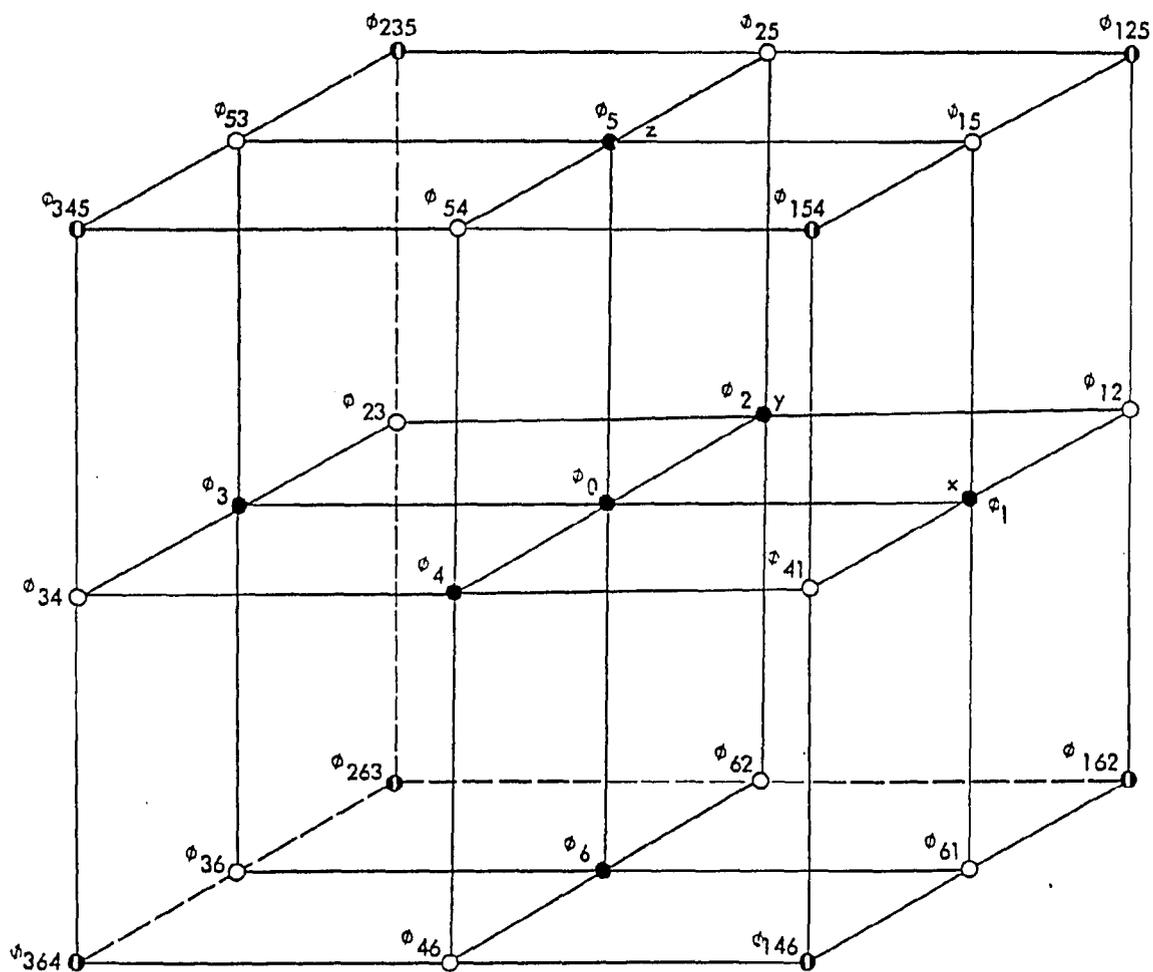


Figure 2. Three-dimensional molecule

will be a factor for the corner nodes and the former will be a factor for the edge nodes. In that respect, as will be shown later, the order of T.E is set up via these parameters. Finally, one should notice that the equation will involve a relationship between planes instead of lines.

With all the foregoing observations, the equivalent relation in 3-D to relation 5 in 2-D, will be the following [16]:

$$(1 - p - p')\phi_N + \frac{P}{4}\phi_E + \frac{P'}{4}\phi_C - (6 - 3p - 4p')\phi_O \quad (6)$$

where:

$$\phi_N = S_{14} + S_{25} + S_{36} \quad (7)$$

$$S_{13} = \phi_1 + \phi_3 = \phi_{i+1,j,k} + \phi_{i-1,j,k} \quad (8)$$

$$S_{24} = \phi_2 + \phi_4 = \phi_{i,j+1,k} + \phi_{i,j-1,k} \quad (9)$$

$$S_{56} = \phi_5 + \phi_6 = \phi_{i,j,k-1} + \phi_{i,j,k+1} \quad (10)$$

and

$$\phi_E = E_1 + E_2 + E_3 \quad (11)$$

$$\begin{aligned} E_1 &= \phi_{12} + \phi_{41} + \phi_{23} + \phi_{34} \\ &= \phi_{i+1,j+1,k} + \phi_{i+1,j-1,k} + \phi_{i-1,j+1,k} + \phi_{i-1,j-1,k} \end{aligned} \quad (12)$$

$$\begin{aligned} E_2 &= \phi_{25} + \phi_{62} + \phi_{54} + \phi_{46} \\ &= \phi_{i,j+1,k+1} + \phi_{i,j+1,k-1} + \phi_{i,j-1,k+1} + \phi_{i,j-1,k-1} \end{aligned} \quad (13)$$

$$\begin{aligned} E_3 &= \phi_{15} + \phi_{53} + \phi_{36} + \phi_{61} \\ &= \phi_{i+1,j,k+1} + \phi_{i+1,j,k-1} + \phi_{i-1,j,k+1} + \phi_{i-1,j,k-1} \end{aligned} \quad (14)$$

and

$$\begin{aligned}
 \phi_C &= \phi_{125} + \phi_{162} + \phi_{154} + \phi_{146} + \phi_{235} + \phi_{263} + \phi_{345} + \phi_{263} \\
 &= \phi_{i+1,j+1,k+1} + \phi_{i+1,j+1,k-1} + \phi_{i+1,j-1,k+1} + \phi_{i+1,j-1,k-1} + \\
 &+ \phi_{i-1,j+1,k+1} + \phi_{i-1,j+1,k-1} + \phi_{i-1,j-1,k+1} + \phi_{i-1,j-1,k-1} \quad (15)
 \end{aligned}$$

III. TECHNICAL DEVELOPMENTS

III.1. Formulation of the Finite Difference

Approximation to the Laplacian Operator

The next step is to relate the derivatives to the respective finite differences. We use the Taylor series to expand each of the function ϕ in equation 6 about the central node (i,j,k) .

To alleviate the derivation, the following differential operators are used:

$$\delta = h_1 \frac{\partial}{\partial x}$$

$$\eta = h_2 \frac{\partial}{\partial y}$$

$$\xi = h_3 \frac{\partial}{\partial z}$$

Thusly, the one-dimensional Taylor theorem could be written as:

$$\phi(x_0 \pm h_1) = (1 \pm \delta + \frac{\delta^2}{2!} \pm \frac{\delta^3}{3!} + \dots) \phi_0 \quad (16)$$

In that manner, equation 8 yields:

$$S_{13} = 2(1 + \frac{\delta^2}{2!} + \frac{\delta^4}{4!} + \frac{\delta^6}{6!} + \dots) \phi_0 \quad (17)$$

Similarly, equations 9 and 10 give:

$$S_{24} = 2(1 + \frac{\eta^2}{2!} + \frac{\eta^4}{4!} + \frac{\eta^6}{6!} + \dots) \phi_0 \quad (18)$$

$$S_{56} = 2(1 + \frac{\xi^2}{2!} + \frac{\xi^4}{4!} + \frac{\xi^6}{6!} + \dots) \phi_0 \quad (19)$$

Moreover, summing equations 17, 18 and 19, one gets:

$$\phi_N = 2 \left[3 + \frac{1}{2!}(\delta^2 + \eta^2 + \xi^2) + \frac{1}{4!}(\delta^4 + \eta^4 + \xi^4) + \frac{1}{6!}(\delta^6 + \eta^6 + \xi^6) \right] \phi_0 + O(h^8) \quad (20)$$

Now, to develop a similar expression for the edge function values that compose equation 11, the Taylor series is written as follows:

$$\phi(x_0 \pm h_1, y_0 \pm h_2) = [1 \pm (\delta \pm \eta) + \frac{1}{2!}(\delta \pm \eta)^2 \pm \frac{1}{3!}(\delta \pm \eta)^3 + \frac{1}{4!}(\delta \pm \eta)^4 + \dots] \phi_0 \quad (21)$$

Therefore, applying equation 21 to each term of equation 12, one gets:

$$\phi_{i+1,j+1,k} = [1 + (\delta + \eta) + \frac{1}{2!}(\delta + \eta)^2 + \frac{1}{3!}(\delta + \eta)^3 + \frac{1}{4!}(\delta + \eta)^4 + \dots] \phi_0, \quad (22)$$

$$\phi_{i+1,j-1,k} = [1 + (\delta - \eta) + \frac{1}{2!}(\delta - \eta)^2 + \frac{1}{3!}(\delta - \eta)^3 + \frac{1}{4!}(\delta - \eta)^4 + \dots] \phi_0, \quad (23)$$

$$\phi_{i-1,j+1,k} = [1 + (-\delta + \eta) + \frac{1}{2!}(-\delta + \eta)^2 + \frac{1}{3!}(-\delta + \eta)^3 + \frac{1}{4!}(-\delta + \eta)^4 + \dots] \phi_0, \quad (24)$$

and

$$\phi_{i-1,j-1,k} = [1 + (-\delta - \eta) + \frac{1}{2!}(-\delta - \eta)^2 + \frac{1}{3!}(-\delta - \eta)^3 + \frac{1}{4!}(-\delta - \eta)^4 + \dots] \phi_0 \quad (25)$$

Finally, summing equations 22-25 and 13, one gets:

$$E_1 = 4 \left[1 + \frac{1}{2!}(\delta^2 + \eta^2) + \frac{1}{4!}(\eta^4 + 6\delta^2\eta^2 + \delta^4) + \frac{1}{6!}(\eta^6 + 15\eta^4\delta^2 + 15\eta^2\delta^4 + \delta^6) + \dots \right] \phi_0, \quad (26)$$

and

$$E_2 = 4 \left[1 + \frac{1}{2!}(\eta^2 + \xi^2) + \frac{1}{4!}(\eta^4 + 6\eta^2\xi^2 + \xi^4) + \frac{1}{6!}(\xi^6 + 15\xi^4\eta^2 + 15\eta^4\xi^2 + \eta^6) + \dots \right] \phi_0 \quad (27)$$

and

$$E_3 = 4 \left[1 + \frac{1}{2!}(\delta^2 + \xi^2) + \frac{1}{4!}(\delta^4 + 6\delta^2\xi^2 + \xi^4) + \frac{1}{6!}(\xi^6 + 15\xi^4\delta^2 + 15\delta^4\xi^2 + \delta^6) + \dots \right] \phi_0 \quad (28)$$

Hence, substituting equations 26-28 into 11, we get:

$$\begin{aligned} \phi_E = & 4 \left[3 + (\delta^2 + \eta^2 + \xi^2) + \frac{2}{4!}(\eta^4 + \delta^4 + \xi^4) + \frac{6}{4!}(\delta^2\eta^2 + \eta^2\xi^2 + \delta^2\xi^2) \right. \\ & + \frac{2}{6!}(\delta^6 + \eta^6 + \xi^6) + \frac{15}{6!}(\delta^4\eta^2 + \delta^4\xi^2 + \eta^4\delta^2 + \eta^4\xi^2 + \xi^4\eta^2 + \xi^4\delta^2) \left. \right] \phi_0 + O(h^8) \end{aligned} \quad (29)$$

Next, to get the expansions of the terms composing equation 15,

Taylor's Theorem in 3-D is used in the following form:

$$\begin{aligned} \phi(x_0 \pm h_1, y_0 \pm h_2, z_0 \pm h_3) = & \left[1 \pm (\delta \pm \eta \pm \xi) + \frac{1}{2!}(\pm \delta \pm \eta \pm \xi)^2 \mp \frac{1}{3!}(\delta \pm \eta \pm \xi)^3 + \right. \\ & \left. + \frac{1}{4!}(\pm \delta \pm \eta \pm \xi)^4 + \dots \right] \phi_0 \end{aligned} \quad (30)$$

This latter equation is applied to each corner point which constitutes equation 15 and in a procedure similar to the above (see Appendix A), one will obtain:

$$\begin{aligned} \phi_C = & 8 \left\{ 1 + \frac{1}{2!}(\delta^2 + \eta^2 + \xi^2) + \frac{1}{4!}(\delta^4 + \eta^4 + \xi^4) + \frac{6}{4!}(\delta^2\eta^2 + \delta^2\xi^2 + \eta^2\xi^2) + \right. \\ & + \frac{1}{6!}(\delta^6 + \eta^6 + \xi^6) + \frac{15}{6!}[\delta^2(\eta^4 + \xi^4) + \eta^2(\delta^4 + \xi^4) + \xi^2(\delta^4 + \eta^4)] + \\ & \left. + \frac{90}{6!} \delta^2\eta^2\xi^2 \right\} \phi_0 + O(h^8) \end{aligned} \quad (31)$$

Substitution of equations 20, 29 and 31 into 6 results in:

$$\begin{aligned}
& (1-p-p')\phi_N + \frac{p}{4}\phi_E + \frac{p'}{4}\phi_C - (6-3p-4p')\phi_O \equiv \{(1-p-p') \\
& [6 + (\delta^2 + \eta^2 + \xi^2) + \frac{1}{12}(\delta^4 + \eta^4 + \xi^4) + \frac{1}{360}(\delta^6 + \eta^6 + \xi^6)] + \\
& + p[3 + (\delta^2 + \eta^2 + \xi^2) + \frac{2}{4!}(\eta^4 + \delta^4 + \xi^4) + \frac{6}{4!}(\delta^2\eta^2 + \eta^2\xi^2 + \delta^2\xi^2) + \\
& + \frac{2}{6!}(\delta^6 + \eta^6 + \xi^6) + \frac{15}{6!}(\delta^4\eta^2 + \delta^4\xi^2 + \eta^4\delta^2 + \eta^4\xi^2 + \xi^4\eta^2 + \xi^4\delta^2) \\
& + 2p'[1 + \frac{1}{2!}(\delta^2 + \eta^2 + \xi^2) + \frac{1}{4!}(\delta^4 + \eta^4 + \xi^4) + \frac{6}{4!}(\delta^2\eta^2 + \delta^2\xi^2 + \eta^2\xi^2) + \\
& + \frac{1}{6!}(\delta^6 + \eta^6 + \xi^6) + \frac{15}{6!}(\delta^2\eta^4 + \delta^2\xi^4 + \eta^2\delta^4 + \eta^2\xi^4 + \xi^2\delta^4 + \xi^2\eta^4) + \\
& + \frac{90}{6!}\delta^2\eta^2\xi^2] - (6-3p-4p')\}\phi_O + O(h^8) \tag{32}
\end{aligned}$$

Grouping like coefficients, simplifying and ordering, the RHS of equation 32 becomes:

$$\begin{aligned}
\text{RHS} = & \{(\delta^2 + \eta^2 + \xi^2) + \frac{1}{12}(\delta^4 + \eta^4 + \xi^4) + \frac{2}{6!}(\delta^6 + \eta^6 + \xi^6) + \\
& + (\frac{p}{4} + \frac{p'}{2})(\delta^2\eta^2 + \eta^2\xi^2 + \delta^2\xi^2) + (\frac{15}{6!}p + \frac{30}{6!}p')[\delta^2\eta^4 + \delta^2\xi^4 + \\
& + \eta^2\delta^4 + \eta^2\xi^4 + \xi^2\delta^4 + \xi^2\eta^4] + \frac{180}{6!}p'\delta^2\eta^2\xi^2\}\phi_O + O(h^8) \tag{33}
\end{aligned}$$

At this stage, an important observation is in order. It concerns the symmetry of the expressions (powers of the differential operators) and since one is only interested in equal spacings, then one can remark the appearance of the Laplacian; i.e., $\delta^2 + \eta^2 + \xi^2 \equiv h^2\nabla^2$. Therefore, one can isolate it in equation 33 as:

$$\begin{aligned}
h^2\nabla^2 = & \{(1-p-p')\phi_N + \frac{p}{4}\phi_E + \frac{p'}{4}\phi_C - (6-3p-4p') - \frac{1}{12}(\delta^4 + \eta^4 + \xi^4) - \\
& - \frac{2}{6!}(\delta^6 + \eta^6 + \xi^6) - (\frac{6p}{4!} + \frac{p'}{2})(\delta^2\eta^2 + \eta^2\xi^2 + \delta^2\xi^2) - \\
& - (\frac{15}{6!}p + \frac{30}{6!}p')[\delta^2\eta^4 + \delta^2\xi^4 + \eta^2\delta^4 + \eta^2\xi^4 + \xi^2\delta^4 + \xi^2\eta^4] - \\
& - \frac{180}{6!}p'\delta^2\eta^2\xi^2\}\phi_O + O(h^8) \tag{34}
\end{aligned}$$

Now, going back to the definition of the difference operators and dividing by h^2 , equation 34 becomes:

$$\begin{aligned}
\nabla^2 \phi_o &= \frac{1}{h^2} [(1-p-p')\phi_N + \frac{p}{4}\phi_E + \frac{p'}{4}\phi_C - (6-3p-4p')\phi_o] \\
&\quad - \left\{ \frac{h^2}{12} [(D_x^4 + D_y^4 + D_z^4) + (\frac{p}{4} + \frac{p'}{2})(D_x^2 D_y^2 + D_x^2 D_z^2 \right. \\
&\quad \left. + D_x^2 D_z^2)] + \frac{h^4}{6!} [2(D_x^6 + D_y^6 + D_z^6) + (\frac{15p}{6!} + \frac{30p'}{6!}) \right. \\
&\quad \left. (D_x^2 D_y^4 + D_x^2 D_z^4 + D_y^2 D_x^4 + D_y^2 D_z^4 + D_z^2 D_x^4) \right. \\
&\quad \left. + \frac{180}{6!} h^4 p' D_x^2 D_y^2 D_z^2 + \dots \right\} \phi_o \tag{35}
\end{aligned}$$

where:

$$D_x = \frac{\partial}{\partial x}, \quad D_y = \frac{\partial}{\partial y}, \quad D_x^2 = \frac{\partial^2}{\partial x^2} \dots$$

The truncation error (T.E) for this relation is determined by the proper choice of the parameters p and p' . It can be seen that the normal seven-point relation occurs for $p = p' = 0$.

III.2. Truncation Error Analysis

III.2.a. The 4th order approximation

For $p = p' = 0$, the F.D equation (35) has a T.E of order 2. In order to get a 4th order T.E, it is necessary to require that:

$$\left[\frac{1}{12} (D_x^4 + D_y^4 + D_z^4) + (\frac{p}{4} + \frac{p'}{2}) (D_x^2 D_y^2 + D_x^2 D_z^2 + D_y^2 D_z^2) \right] \phi_o \equiv 0 \tag{36}$$

To ease the developments, the following definitions, for operator identities, are introduced:

$$\begin{aligned}
h^2 \left(\frac{\partial^2}{\partial x \partial y} + \frac{\partial^2}{\partial y \partial z} + \frac{\partial^2}{\partial z \partial x} \right) &\equiv h^2 (D_{xy} + D_{yz} + D_{zx}) \\
&\equiv h^2 (D)_{ij} \tag{37}
\end{aligned}$$

Therefore, define:

$$(D^2)_{ij} \equiv (D_{xy}^4 + D_{yz}^4 + D_{zx}^4) \quad (38)$$

Furthermore:

$$\begin{aligned} h^4 \nabla^4 &\equiv (h^2 \nabla^2)^2 \equiv (\delta^2 + \eta^2 + \xi^2)^2 \\ &\equiv h^4 (D_x^4 + D_y^4 + D_z^4) + 2h^4 (D^2)_{ij} \end{aligned} \quad (39)$$

Hence, equation 36 becomes:

$$\left\{ \frac{1}{12} [\nabla^4 - 2(D^2)_{ij}] + \left(\frac{p}{4} + \frac{p'}{2} \right) (D^2)_{ij} \right\} \phi_o \equiv 0$$

or

$$[\nabla^4 + (-2 + 3p + 6p') (D^2)_{ij}] \phi_o \equiv 0 \quad (40)$$

Equation 36 is indeterminable, since it contains two unknowns, p and p' . One has, then, to choose arbitrarily one of the parameters and solve for the other.

Let $p' = 0$. Then, from equation 40:

$$p = \frac{2}{3} - \frac{\nabla^4 \phi_o}{3(D^2)_{ij} \phi_o} \quad (41)$$

and if $p = 0$, then from equation 41:

$$p' = \frac{1}{3} - \frac{\nabla^4 \phi_o}{6(D^2)_{ij} \phi_o} \quad (42)$$

At this point, two useful remarks are appropriate to mention. First, when one uses the parameter p given by equation 41; i.e., $p' = 0$, then from equation 35, the corner points are not needed in the Laplacian evaluation. For this case, the 4th order approximation uses

the normal seven points and the 12 edges points in equation 35. Therefore, in this study it will be called the "Nineteen-Point Formula." Similarly, if one uses the value of the parameter p' , given by equation 42, the edge points are not needed in the Laplacian determination (equation 35). It will be called the "Fifteen-Point Formula."

Second, in terms of effecting a numerical solution, the mixed derivative terms (denominator of equations 41 and 42) cannot be evaluated. However, it may be feasible to use numerical approximations calculated from the solution for these terms. This results in a nonlinear solution. Since

$$h^4(D^2)_{ij}\phi_o \equiv \left(\frac{\partial^4}{\partial x^2\partial y^2} + \frac{\partial^4}{\partial y^2\partial z^2} + \frac{\partial^4}{\partial z^2\partial x^2}\right)\phi_o,$$

we can use (Appendix A)

$$(D^2)_{ij}\phi_o = \frac{1}{h^4}[\phi_E - 4\phi_N + 2\phi_o] + O(h^2) \quad (43)$$

where ϕ_E and ϕ_C are given by equations 11 and 15, respectively.

Note that this approximation is obtained by the appropriate elimination between equations 11 and 15.

III.2.b. The 6th order approximation

To get a 6th order T.E for the Laplacian, in addition to equation 40, written here again,

$$[\nabla^4 + (-2 + 3p + 6p')(D^2)_{ij}]\phi_o \equiv 0 \quad (44)$$

one needs to require

$$\begin{aligned} & [2(D_x^6 + D_y^6 + D_z^6) + (15p + 30p')(D_x^2D_y^4 + D_x^2D_z^4 + D_y^2D_x^4 + \\ & + D_y^2D_z^4 + D_z^2D_x^4 + D_z^2D_y^4)]\phi_o \equiv 0 \end{aligned} \quad (45)$$

Here again the following relationships will be needed to solve equation 45. First, by definition of the difference operators and using

equations 37 and 38, one writes:

$$\delta\eta\xi \equiv h^3 D_{xyz}$$

and

$$\delta^2 \eta^2 \xi^2 \equiv h^6 D_{xyz}^2 \quad (46)$$

Also,

$$\begin{aligned} h^6 \nabla^2 (D^2)_{ij} &\equiv (\delta^2 + \eta^2 + \xi^2) (\delta^2 \eta^2 + \delta^2 \xi^2 + \eta^2 \xi^2) \\ &\equiv \delta^2 (\eta^4 + \xi^4) + \eta^2 (\delta^4 + \xi^4) + \xi^2 (\delta^4 + \eta^4) + 3h^6 D_{xyz}^2 \end{aligned}$$

Therefore,

$$h^6 \Delta^6 \equiv (h^2 \nabla^2)^3 \equiv h^6 (D_x^6 + D_y^6 + D_z^6) + 3h^6 \nabla^2 (D^2)_{ij} - 3h^6 D_{xyz}^2 \quad (47)$$

Using equation 47, equation 45 gives:

$$[\nabla^6 + (-3 + \frac{15}{2}p + 15p') \nabla^2 (D^2)_{ij} + (3 - \frac{45}{2}p + 45p') D_{xyz}^2] \phi_0 \equiv 0 \quad (48)$$

The system of equations 44 and 48 is the one to be solved for p and p' .

These are determined in Appendix B, to be:

$$p \equiv \frac{2}{5} - (B + A) \quad (49)$$

and

$$p' \equiv \frac{2}{15} + \frac{1}{2}(A - B) \quad (50)$$

where

$$A \equiv \frac{1}{90} \frac{[2\nabla^6 \phi_0 + (4 - 5 \frac{\nabla^4 \phi_0}{(D^2)_{ij} \phi_0} \nabla^2 (D^2)_{ij} \phi_0]}{D_{xyz}^2 \phi_0} \quad (51)$$

and

$$B \equiv \frac{1}{6} \left[\frac{\nabla^4 \phi_0}{(D^2)_{ij} \phi_0} \right] \quad (52)$$

Here again, a numerical approximation is needed so that equations 49 and 50 can be evaluated.

In addition to equation 43, one introduces:

$$h^6 D_{xyz}^2 \phi_0 \equiv \frac{\partial^6}{\partial x^2 \partial y^2 \partial z^2} \phi_0$$

or, a numerical approximation is (Appendix C):

$$D_{xyz}^2 \phi_0 \equiv \frac{1}{h^6} [\phi_C - 2\phi_E + 4\phi_N - 8\phi_0] + O(h^2) \quad (53)$$

where ϕ_N , ϕ_E and ϕ_C are defined by equations 15, 11 and 7, respectively.

Here again, equation 53 is obtained if one eliminates all the terms in equations 7, 11 and 15 except the $D_{xyz}^2 \phi_0$ term (see Appendix C).

Before proceeding further, the following remarks are in order. First, it's not immediately apparent what the effects in the above approximations (equations 43 and 53) would have on the truncation error. However, the error term from these equations should appear as a secondary form. Second, as was mentioned by Eckholtz [13], this type of estimation "acted to reduce the overall truncation error as well as simplifying the application of the technique." Finally, it is worth noticing that only the mesh values needed in the basic equation (35) are called for in these approximations.

IV. COMPUTATIONAL PROCEDURE

IV.1. The Analytical Solution

Considering a cubical domain (reactor) $L \times L \times L$, the reactor equation (4) is easily solved by the separation of variables method:

$$\nabla^2 \phi + B^2 \phi = 0 \quad (4)$$

For this type of reactor, the flux must vanish at the extrapolated distance, L . So the boundary conditions for equation 4 are:

$$\phi(x, y, z) \Big|_{\text{external surfaces}} \equiv 0 \quad (54)$$

Let

$$\phi \equiv \phi(x, y, z) \equiv X(x) \cdot Y(y) \cdot Z(z) \quad (55)$$

Substituting this into equation 4 gives:

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} + B^2 \right) X(x) \cdot Y(y) \cdot Z(z) = 0 \quad (56)$$

which, after expansion and simplification, yields:

$$\frac{1}{X(x)} \frac{d^2}{dx^2} X(x) + \frac{1}{Y(y)} \frac{d^2 Y(y)}{dy^2} + \frac{1}{Z(z)} \frac{d^2 Z(z)}{dz^2} + B^2 \equiv 0 \quad (57)$$

Solving, as usual, for each function, then applying equation 54 and taking the fundamental harmonic, one obtains the flux:

$$\phi(x, y, z) \equiv C \sin \frac{\pi x}{L} \sin \frac{\pi y}{L} \sin \frac{\pi z}{L} \quad (58)$$

where;

$$B^2 = \frac{3\pi^2}{L} \quad (59)$$

and L is the cube dimension. Finally, C is a normalization constant which can be found once the total power is known. For the case at hand, it will be taken equal to unity.

IV.2. Definition of Error and Speed of Convergence

In addition to the truncation error described previously, other types of error exist such as boundary and round-off errors. The combination of T.E and boundary error is called the discretization error [45]. Nevertheless, in this comparative study no concern is given to all the above errors. One is primarily interested in the relative difference between two solutions, the analytical (ANAL) and the numerical (FD) solutions.

The relative error is defined by:

$$E_{R_{ijk}} = \frac{\|\phi - \phi^*\|}{\phi^*} \Big|_{ijk} \quad (59)$$

where ϕ and ϕ^* are the numerical values of the FD and ANAL solutions. Note that these functions are computed at each node (i,j,k) . Since all norms on R^n are equivalent with respect to convergence, in this study $\|\cdot\|$ represents the Euclidian norm defined as [47]:

$$L2NORM = \left[\sum_{ijk} \|\phi - \phi^*\|^2 \right]^{1/2} \quad (60)$$

Furthermore, the effectiveness of a method can only be efficiently determined through the use of the number of iterations and the work required per iteration. For this, the following definition of the

rate of convergence is introduced [48]:

$$v = - \ln \lambda_1 \quad (61)$$

where:

v = convergence rate, and

λ_1 = largest eigenvalue of the iteration matrix.

The parameter λ_1 can be approximated by using the ratio of two successive residual vectors, so that:

$$\lambda_1 \approx \frac{\|\underline{r}^{\ell+1}\|}{\|\underline{r}^{\ell}\|} \quad (62)$$

where \underline{r} is the residual vector defined by:

$$\underline{r} = \underline{X}^{\ell+1} - \underline{X}^{\ell} \quad (63)$$

and \underline{X} is either the FD or ANAL solution and ℓ is the iterate number.

IV.3. The Successive Overrelaxation Method (SOR)

The general form of the iterative process is given by:

$$\phi^{(\ell+1)} = \phi^{\text{cal}}_{\alpha} + (1-\alpha)\phi^{\ell} \quad (64)$$

where ϕ^{cal} = the value of ϕ calculated using the Gauss-Seidel method.

Here, it will be estimated using the six neighboring points (equation 35) with the appropriate expressions for the parameters p and p' ;

α = relaxation parameter; and

ϕ^{ℓ} = the value of ϕ from the previous iteration.

A major problem associated with the use of the SOR is the determination

of the optimal relation factor, α_m [49]. In spite of this, some optimization will be undertaken later.

IV.4. Calculation Description

A short description of the overall calculation will be given here. More specific information about every solved problem will be presented later (Chapter V).

To investigate the higher order models, several problems are solved. The computer program, designed and written for this purpose, is very similar to any standard F.D one, with the exception of the parameters (p and p') calculation. To ease any future program's adaptability and updating, most of the computation is done by the sub-routines.

The analytical solution (ANAL) is calculated using equation 58. For the eigenvalue, equation 59 is used. The numerical solution (F.D) is determined by solving equation 35, with the appropriate values of p and p' given by equations 41, 42, 45 and 50. Moreover, to judge the models' performances, the Euclidian Norm (equation 60) for the solution and the rate of convergence given by equation 61 are calculated. Finally, since the numerical calculation is iterative, one needs an initial guess to begin it.

A constant function of unity is assumed initially. However, these conditions or others might cause some hidden problems, such as that revealed by Bartal et al. [39, 40].

This prompted the author to be more cautious in determining at which

iteration the calculation of the parameters (p and p') should start. This is also due to the fact that the solution depends on these parameters and vice versa, which might result in instabilities. Again, more will be said later about this important aspect.

V. RESULTS AND DISCUSSION

V.1. The Eigenvalue Problem

Here equation 4

$$\nabla^2 \phi + B^2 \phi = 0 \quad (65)$$

will be solved with the condition:

$$\phi(x_i, y_j, z_k) \Big|_{x_i, y_j, z_k \text{ on boundary}} = 0 \quad (66)$$

The eigenvalue B^2 and the eigenfunction ϕ will be evaluated at each node (x_i, y_j, z_k) numerically using equations 35 and 4, then compared to their corresponding values given by equations 58 and 59, respectively.

V.1.a. The eigenvalue evaluation

Table 1 lists the values of B^2 and the CPU time of the calculation for different mesh sizes for the three methods.

The absolute and relative errors are shown in Figures 3-5. As expected, the 6th order (27-point) outperforms, in accuracy and efficiency, all the lower order approximations. In considering the usual 7-point method, one should use at least 13 nodes per side in order to get the same accuracy obtained when using the 27-point with 4 nodes (just 2 interior nodes) (see Figures 3-5). This fact illustrates well the memory savings. The efficiency of the models is described in Figure 6. The maximum absolute error is plotted versus the total time required for convergence. As one can see, for a lower number of grid points

Table 1. B^2 value for the eigenvalue problem

Step size	Total no. of grids	Analytical B2AN	7-point			15-point		
			Time (sec)	B^2	Relative error (%)	Time (sec)	B^2	Relative error (%)
0.3333	4	29.608813	2	26.99990	8.81	2	30.29525	2.31
0.2	6	29.608813	3	28.64744	3.25	5	29.69133	0.28
0.16666	7	29.608813	6	28.93850	2.26	11	29.64770	0.13
0.125	9	29.608813	16	29.23024	1.28	47	29.62080	0.04
0.1	11	29.608813		29.36600	0.81	135	29.61367	0.016
0.0833	13	29.608813	104	29.44000	0.57	342	29.61119	0.0078

19-point			27-point		
Time (sec)	B^2	Relative error (%)	Time (sec)	B^2	Relative error (%)
2	31.65134	6.9	2	29.25165	1.2
5	29.77985	0.57	5	29.59613	0.043
12	29.68613	0.26	12	29.60475	0.01
49	29.63186	0.078	49	29.60811	0.002
144	29.61799	0.031	138	29.60860	0.0006
358	29.61315	0.01	357	29.60879	0.0003

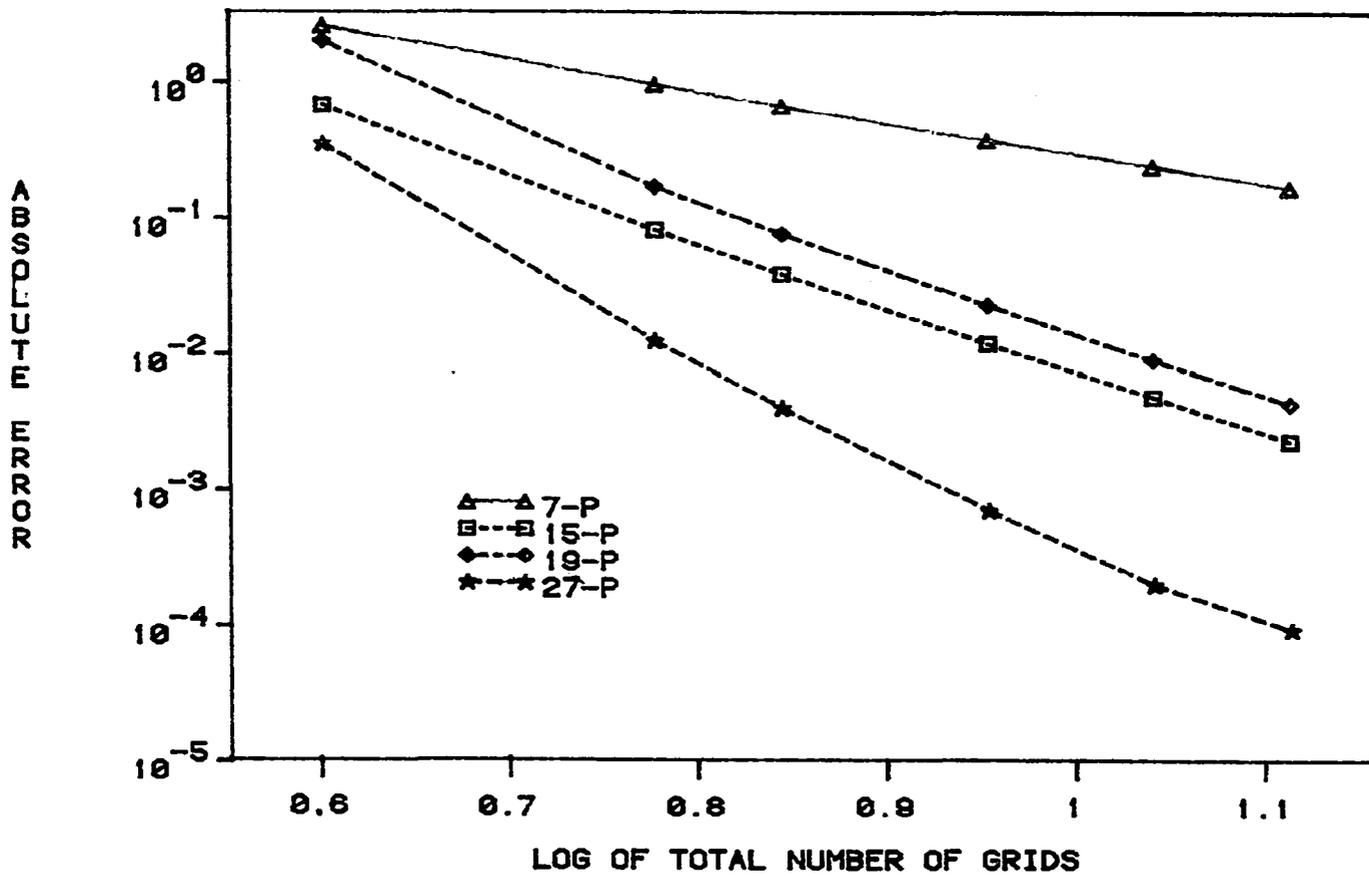


Figure 3. Maximum absolute error of B^2 for the eigenvalue problem as a function of the total number of grids

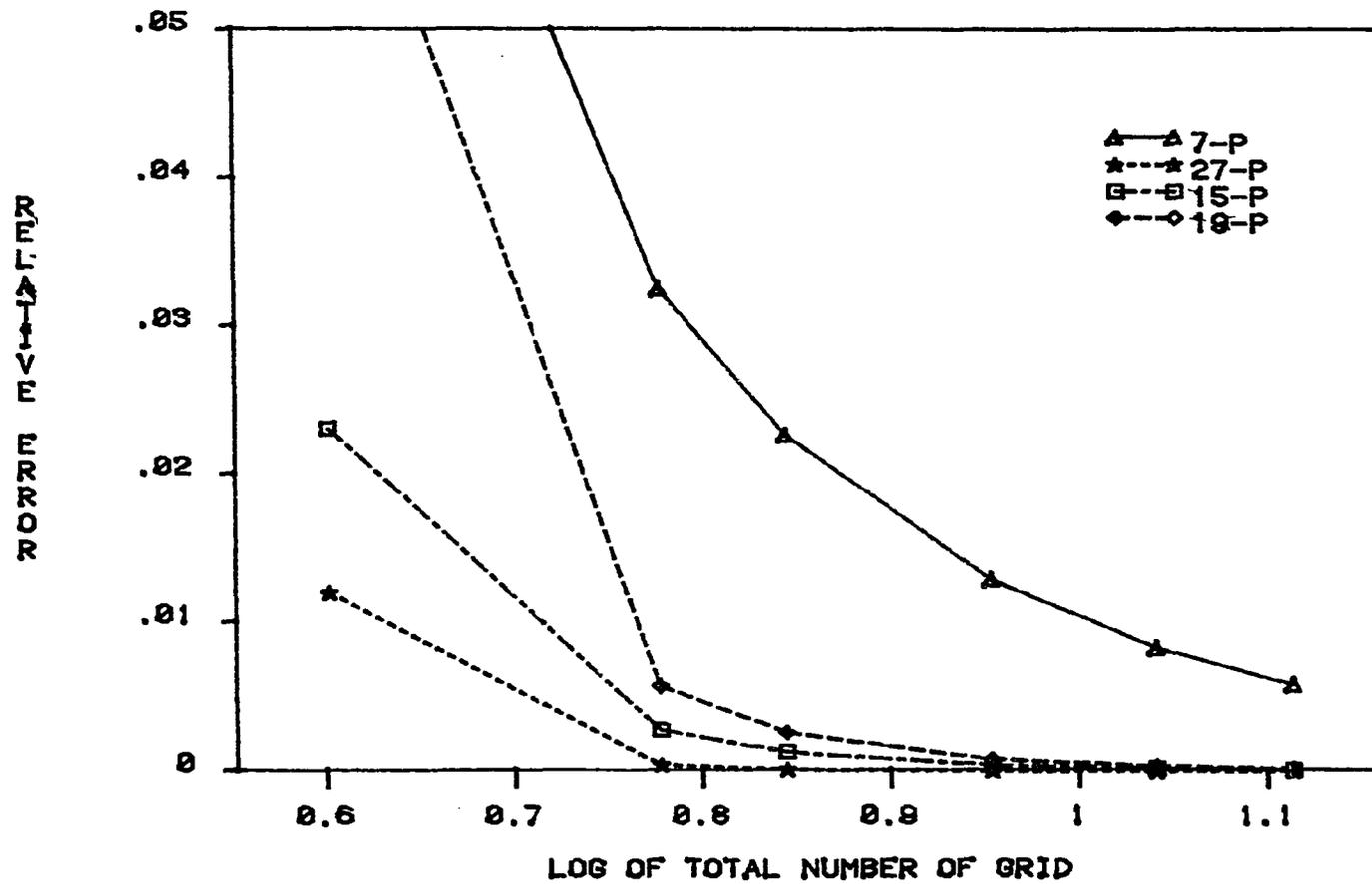


Figure 4. Relative error of B^2 for the eigenvalue problem as a function of the logarithm (of the total number of grids)

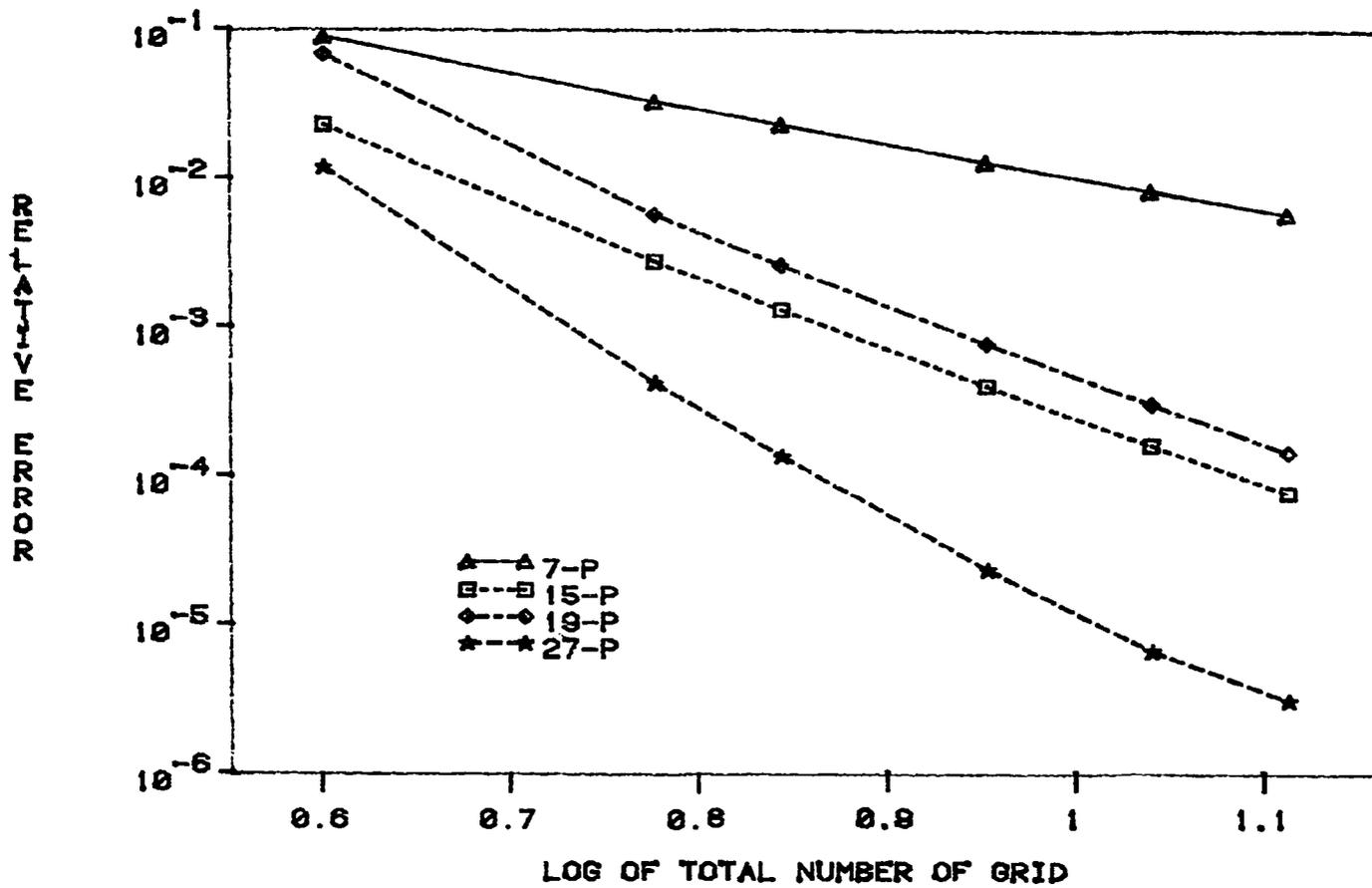


Figure 5. Relative error of B^2 as a function of the logarithm (of the total number of grids)

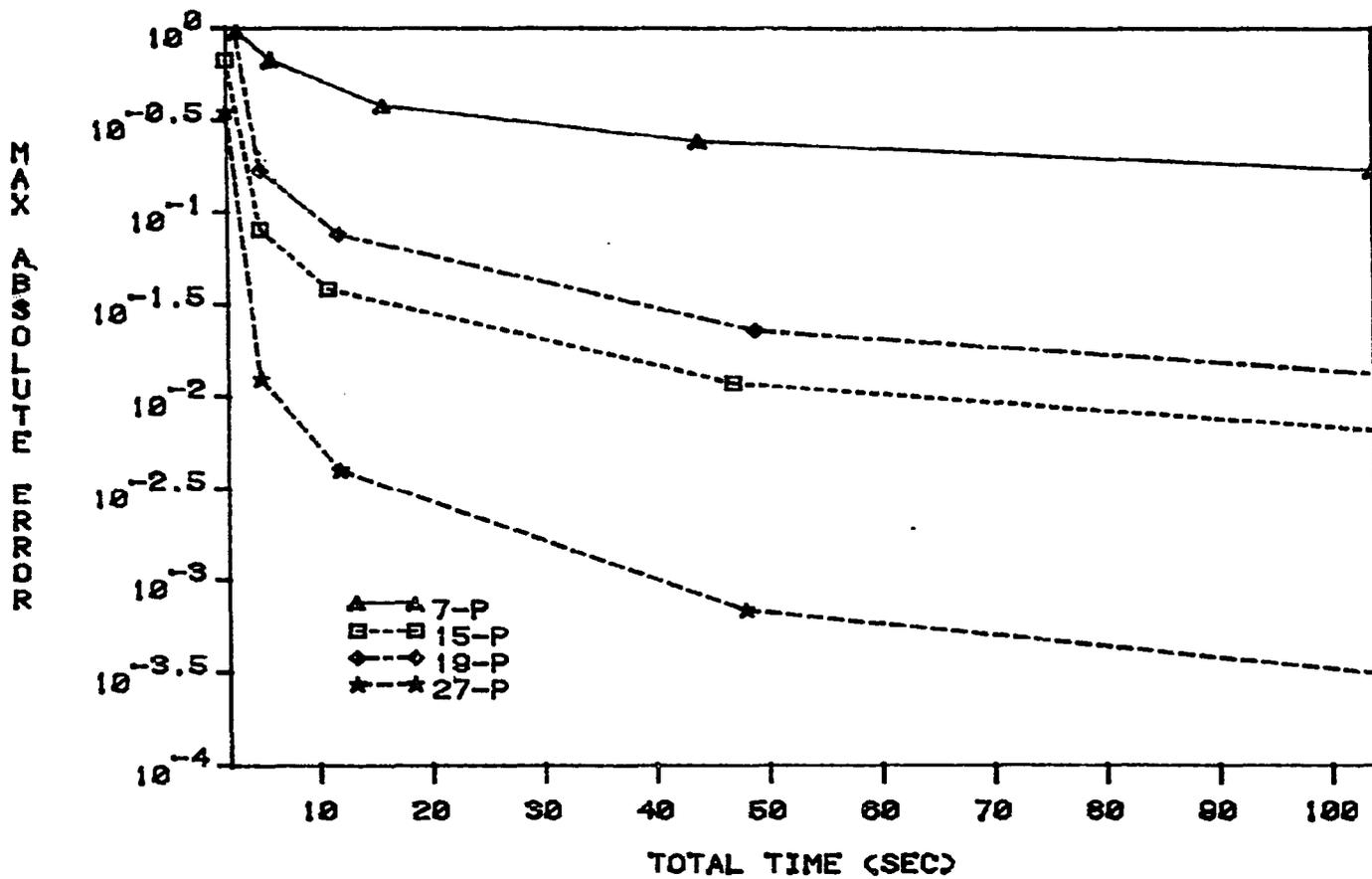


Figure 6. Maximum absolute error of B^2 for the eigenvalue problem as a function of the total time needed for convergence

(up to nine per side), all methods required the same CPU time. However, only the higher order ones lessened the error perceptively, especially the 27-point method which reduced the error to about 0.001.

A similar conclusion is drawn from Figure 7, where the error is plotted as a function of the number of iterations needed to achieve convergence. For less than 50 iterations (without any relaxation), the 6th order diminished the error to less than 0.001.

All the numerical results of this section demonstrate the computational efficiency when using any of the higher order finite difference methods to evaluate the eigenvalue.

V.1.b. The eigenfunction comparison

As one can see from Figure 8, the 7-point and 27-point results are very close to the analytical solution. In other words, the superiority of the higher order approximations isn't as apparent as was previously found. However, this is expected in solving an eigenvalue problem and normalizing the solution.

V.1.c. The order of the truncation error

Before proceeding further, verification of the order of the T.E for all four methods will be made. To do so, the following relation is considered:

$$T.E = O(h^n) \quad (67)$$

where n is the order of the T.E and h is the step size. To determine n from the numerical results, equation 67 is written [46]

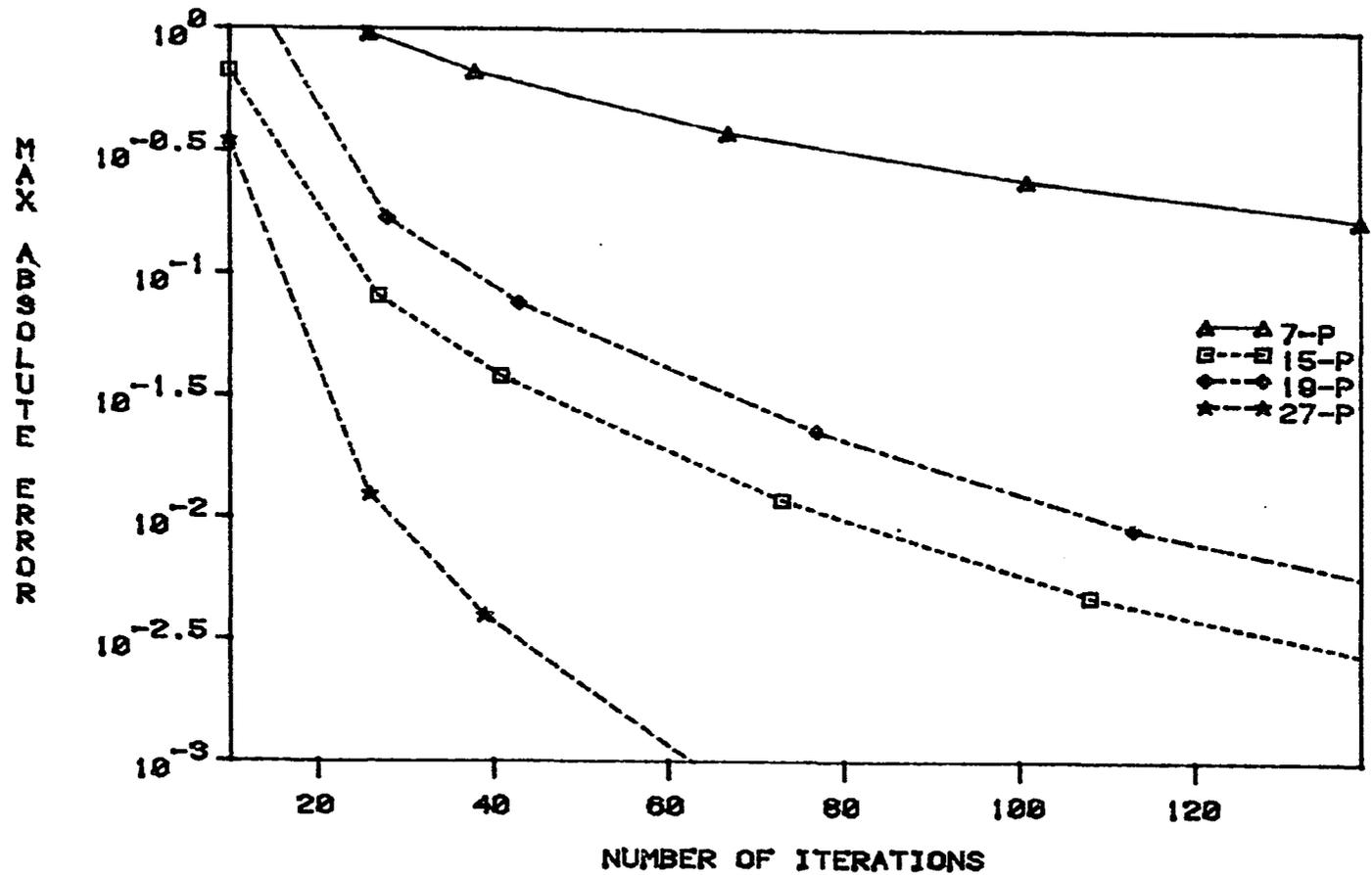


Figure 7. Maximum absolute error (log scale) on B^2 as a function of the total number of iterations needed for convergence

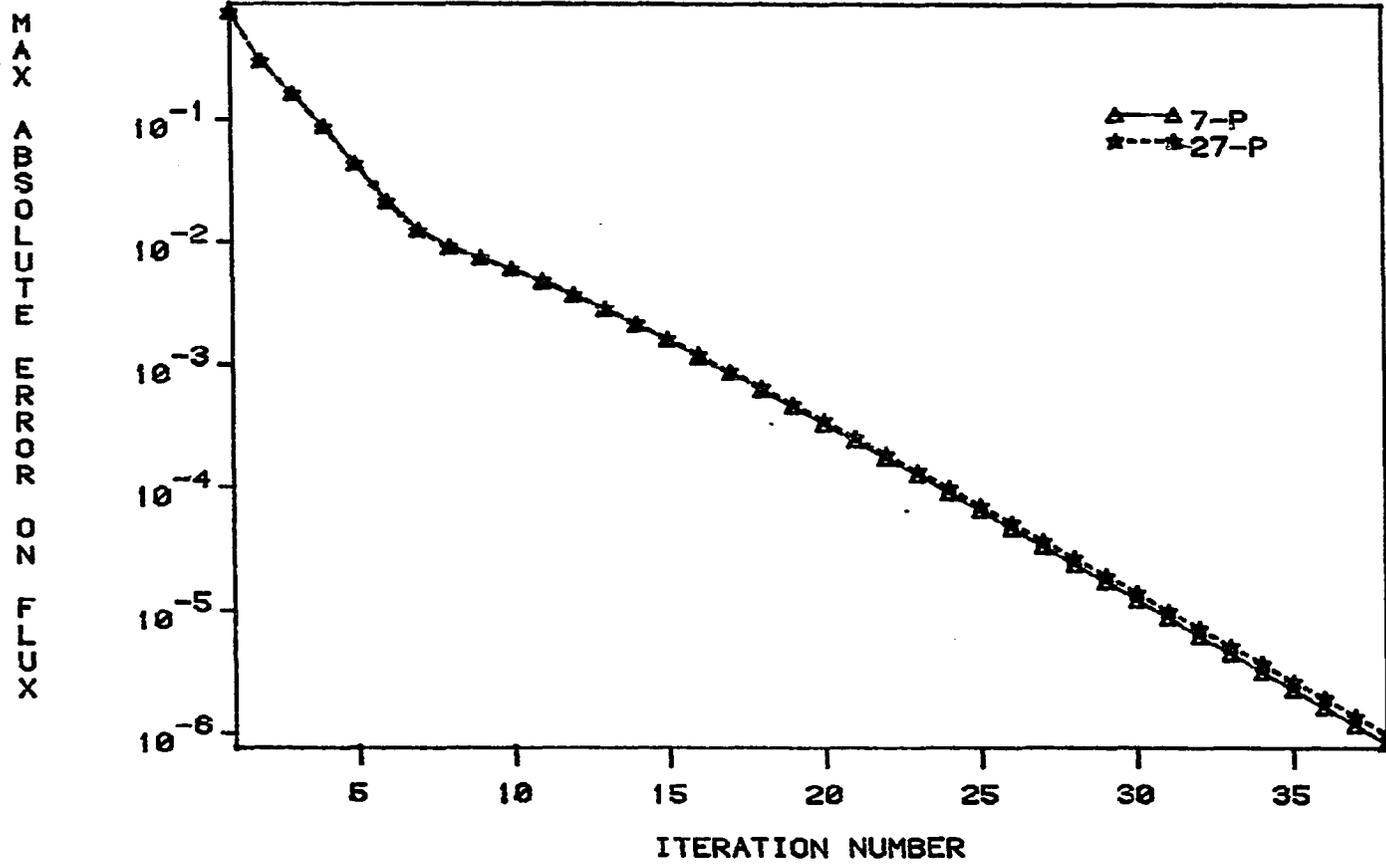


Figure 8. Maximum absolute error on the eigenfunction for the eigenvalue problem as a function of the number of iterations needed for convergence

as:

$$\text{Error} = O(h^n) = Ah^n \quad (68)$$

so that:

$$\text{Log (error)} = \log A + n \log h \quad (69)$$

Since one is comparing different computational methods, one is interested in slopes of equation 69.

$$\text{Log (error)} = n \log h \quad (70)$$

Therefore, the slope of the logarithm of the error versus the logarithms of spacing will result in the value of n . This is shown in Figure 9. The measured slopes agree well with the expected values of 2, 4 and 6.

At this stage, two remarks are in order. First, as can be verified from the graph, the 15-P and 19-P lines both have a slope of "around" 4. However, the fact that they don't coincide is due to the constant A defined in equations 68-69, which seems to be greater for the 19-point relation. Second, the 27-P line has a little curvature at the lower left. This is a characteristic of the round-off errors, which started to grow as the mesh size is refined.

V.1.d. Verification procedure

Another characteristic of the present model is the ability to check the credibility of its solution against established solutions. This might be of great advantage in any real situation where the analytical

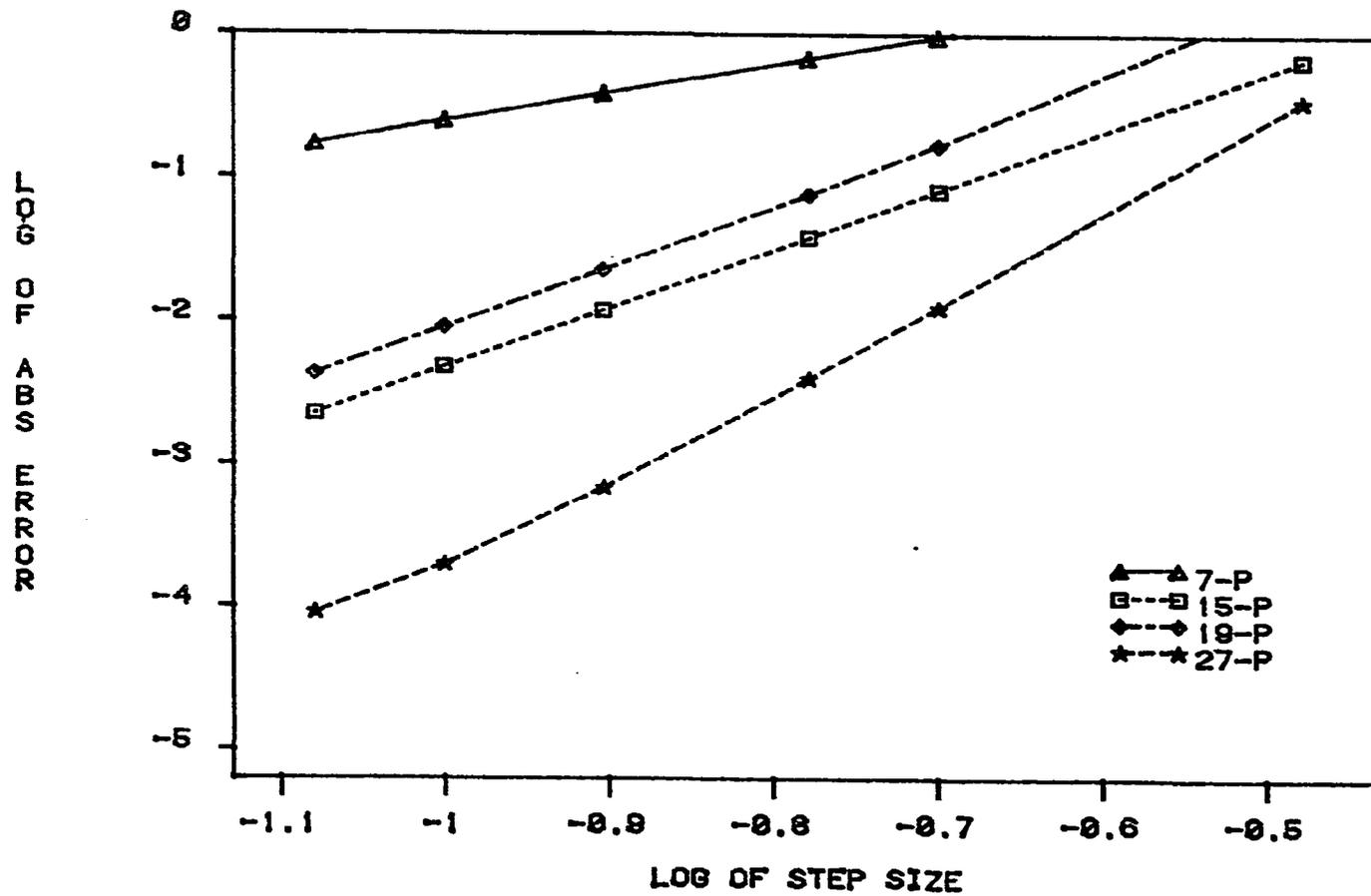


Figure 9. Maximum absolute error of B^2 for the eigenvalue problem as a function of the logarithm of the mesh size

solution is unknown. For example, if p or p' or (p and p') are set to zero, then each of the high order approximations will yield the same results as the usual 7-point. This has been performed for every scheme and for different step sizes.

Moreover, for the eigenvalue problem, the analytical solution is known. Therefore, one will use it to verify the expressions of the mixed operators $(D^2)_{ij}$ (Appendix B) and $(D^2)_{xyz}$ (Appendix D) and also the values of the parameters p and p' (equations 42, 45 and 50).

As mentioned in Appendix B, two relations for the operator $(D^2)_{ij}$ were found. Expression XI-8 was selected, since it uses fewer points. To validate this selection and its effect on the overall calculations and on the values of the parameters p and p' , several experiments were performed using equations XI-7 and XI-8. The results are shown in Tables 2 and 3.

For the mixed operator $(D^2)_{ij}$, as one can observe from Table 2, expression XI-8 produced much better results. The average difference between the numerical and analytical values is about 4.4%. This engendered a difference of 14.5% for p and p' corresponding to the 4th order T.E, whereas for the 6th order T.E, the dissimilarities were of 7.7% to 10.6% for p and p' , respectively. On the other hand, from Table 3, the difference between the numerical and analytical values for $(D^2)_{xyz}$ is about 6.6% using either formula. Finally, from Table 2 one can notice that the eigenvalue is also better when obtained using XI-8 for $(D^2)_{ij}$.

All of the above results support what was mentioned previously, that

Table 2. Analytical and numerical values for the 4th order mixed operator and the parameters p and p'

Model	Node i= j=k	Analytical			$(D^2)_{ij}$ given by XI-8						
		$(D^2)_{ij}$	p	p'	$(D^2)_{ij}$	Relative error (%)	p	Relative error (%)	p'	Relative error (%)	B ²
15-P	2	36.52841		-0.166667	34.8905	4.48			-0.191507	14.9	29.6477
	3	189.8072		-0.166667	181.30833	4.47			-0.191478	14.8	
	4	292.2773		-0.166667	279.14621	4.48			-0.191472	14.9	
	5	189.8072		-0.166667	181.31087	4.48			-0.191473	14.8	
	6	36.52840		-0.166667	34.89318	4.70			-0.191474	14.8	
19-P	2		-0.33333		34.8904	4.40	-0.385742	15.7			29.6813
	3		-0.33333		181.3082	4.47	-0.385679	15.6			
	4		-0.33333		279.1460	4.47	-0.385668	15.7			
	5		-0.33333		181.3108	4.48	-0.385669	15.7			
	6		-0.33333		34.8931	4.70	-0.385672	15.7			
27-P	2		0.4000	-0.36666	34.8909	7.79	0.431180	7.79	-0.405570	10.60	29.6048
	3		0.4000	-0.36666	181.3086	7.77	0.431111	7.77	-0.405511	10.59	
	4		0.4000	-0.36666	279.1461	7.77	0.431105	7.77	0.405506	10.59	
	5		0.4000	-0.36666	181.3108	7.77	0.431106	7.77	0.405507	10.59	
	6		0.4000	-0.36666	34.8931	7.79	0.431107	7.79	-0.405508	10.60	

Table 2. (Continued)

Model	Node i=j=k	$(D^2)_{ij}$ given by XI-7					B^2	
		$(D^2)_{ij}$	Relative error (%)	p	Relative error (%)	p'		Relative error (%)
15-P	2	31.7743	13			-0.25168	51.0	29.870
	3	165.1140	13			-0.25164	50.9	
	4	254.2139	13			-0.25163	50.9	
	5	165.1169	13			-0.25164	50.9	
	6	31.7766	13			-0.25164	50.9	
19-P	2	31.774	13	-0.507380	52.2			29.92193
	3	165.114	13	-0.507321	52.1			
	4	254.213	13	-0.507307	52.2			
	5	165.116	13	-0.507308	52.1			
	6	31.776	13	-0.50731	52.1			
27-P	2	31.7743	13	0.426860	6.71	-0.463417	26.36	29.8273
	3	165.1143	13	0.426761	6.69	-0.46333	26.36	
	4	254.2139	13	0.426756	6.69	-0.463326	26.36	
	5	165.1169	13	0.426757	6.69	-0.463327	26.36	
	6	31.7766	13	0.426758	6.71	-0.46333	26.36	

Table 3. Analytical and numerical values for the 6th order mixed operator

Node I=J=K	Analytical	D2IJ given by XI-8	Relative error (%)	D2IJ given by XI-7	Relative error (%)
2	-120.1737	-112.1779	6.65	-112.1721	6.65
3	-624.4407	-582.9744	6.64	-582.9710	6.66
4	-961.3893	-897.5642	6.63	-897.5648	6.63
5	-624.4406	-582.9847	6.64	-582.9849	6.64
6	-120.1736	-112.1952	6.65	-112.1952	6.65

the effects of using a numerical approximation of 2nd order for the mixed operators will be secondary and are still consistent with the higher order model.

V.2. The Boundary Value Problems

As stated in Section V.1.b, the performance of the higher order approximations was clearly shown through the behavior of the error on the computation of the eigenvalue. Unfortunately, due to the nature of the problem being solved, the eigenfunctions did not show noticeable dissimilarities. This stimulated the need to study other boundary value problems. However, to examine the obtained solutions, no closed form is available. The alternatives were to determine or establish a boundary value problem from a known analytical solution or to use a very fine mesh solution as the benchmark. Here, the latter is used. The former will be analyzed in the next paragraph.

V.2.a. The Dirichlet problem

The equation to be considered is also given by equation 4; i.e.,

$$\nabla^2 \phi + B^2 \phi \equiv 0 \quad (4)$$

where, from the one group reactor equation:

$$B^2 \equiv -\Sigma_a + \frac{1}{\lambda} \nu \Sigma_f$$

So, equation 4 becomes:

$$\nabla^2 \phi + \left(-\Sigma_a + \frac{1}{\lambda} \nu \Sigma_f\right) \phi = 0 \quad (71)$$

where:

$\lambda \equiv$ effective neutron multiplication factor,

$\Sigma_a =$ absorption cross-section, and

$\nu \Sigma_f \equiv$ fission cross-section.

Equation 71 will be solved for different nonzero boundary conditions as an external source problem and a given value of λ . Using the data of Table 4, Figures 10-13 illustrate the maximum absolute error on the flux versus the number of iterations needed for convergence.

Table 4. Data for the Dirichlet problem

Σ_a	0.08
$\Sigma \nu_f$	0.135
λ	1.2, 0.2
Boundary value	1.0 (on all external surfaces)
Number of grids per side	4, 7, 11, 13

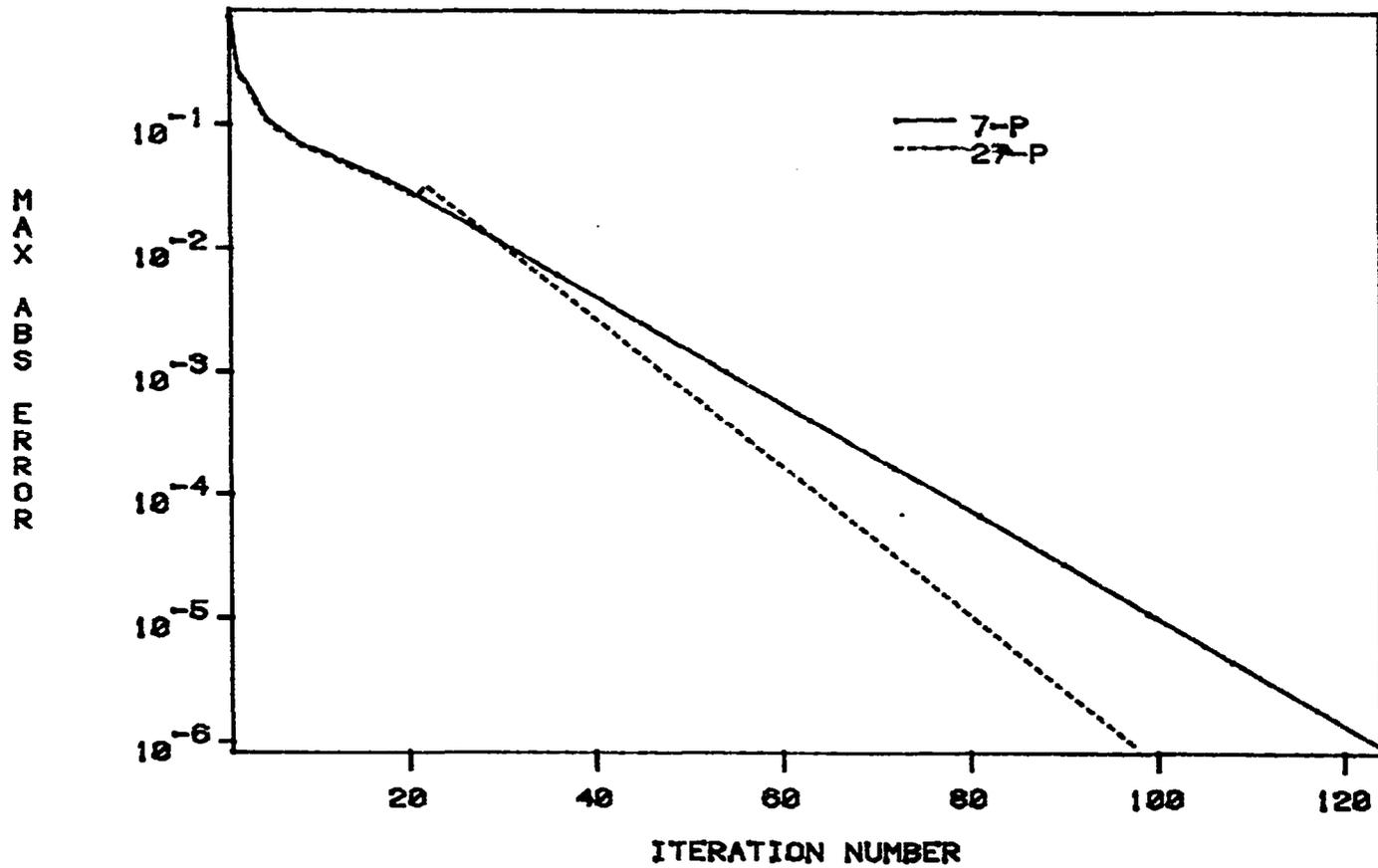


Figure 10. Maximum absolute error on ϕ for Dirichlet problem as a function of the number of iterations (step size of 0.1, $\lambda = 1.2$)

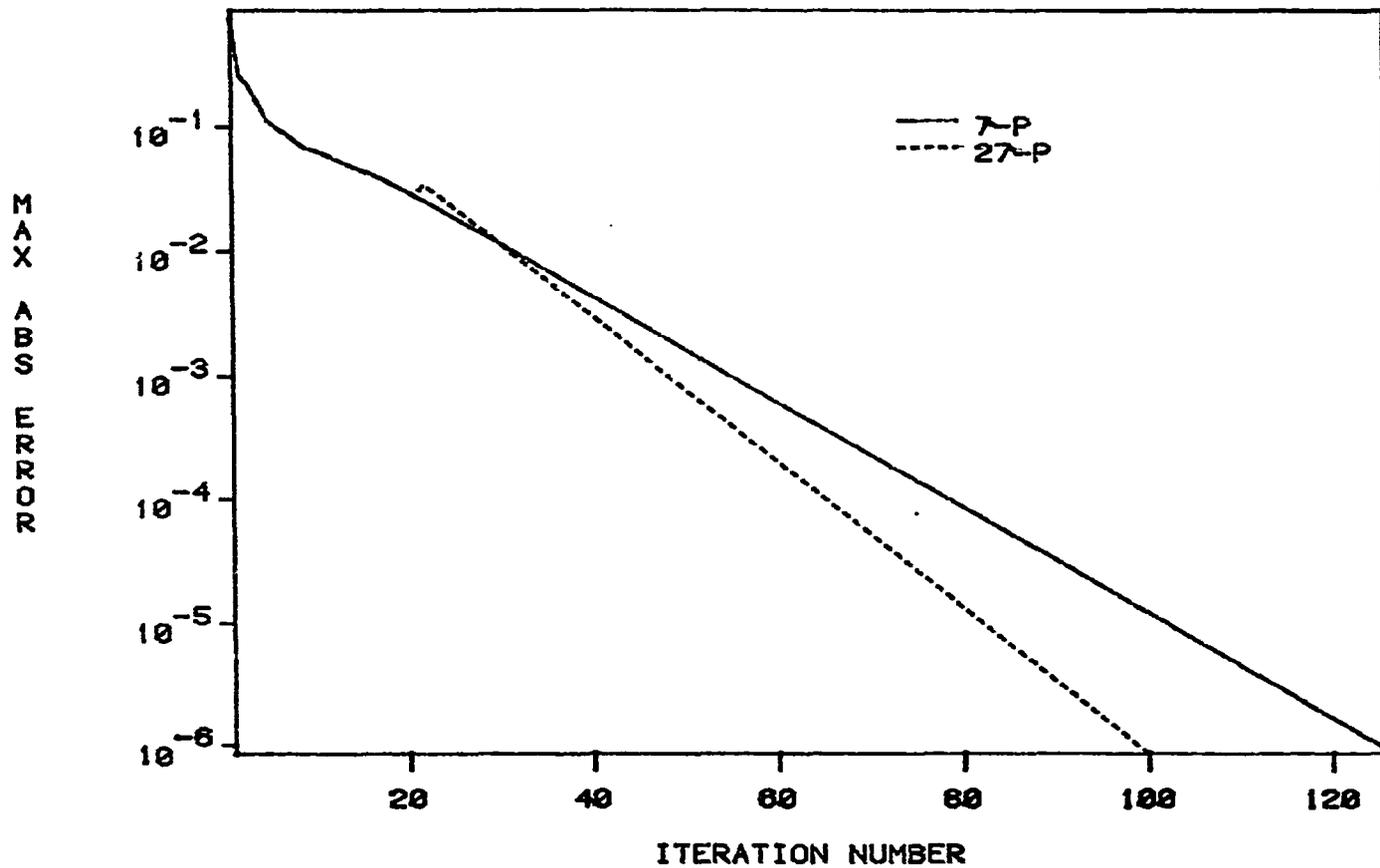


Figure 11. Maximum absolute error on ϕ for Dirichlet problem as a function of the number of iterations (step size of 0.1, $\lambda = 0.2$)

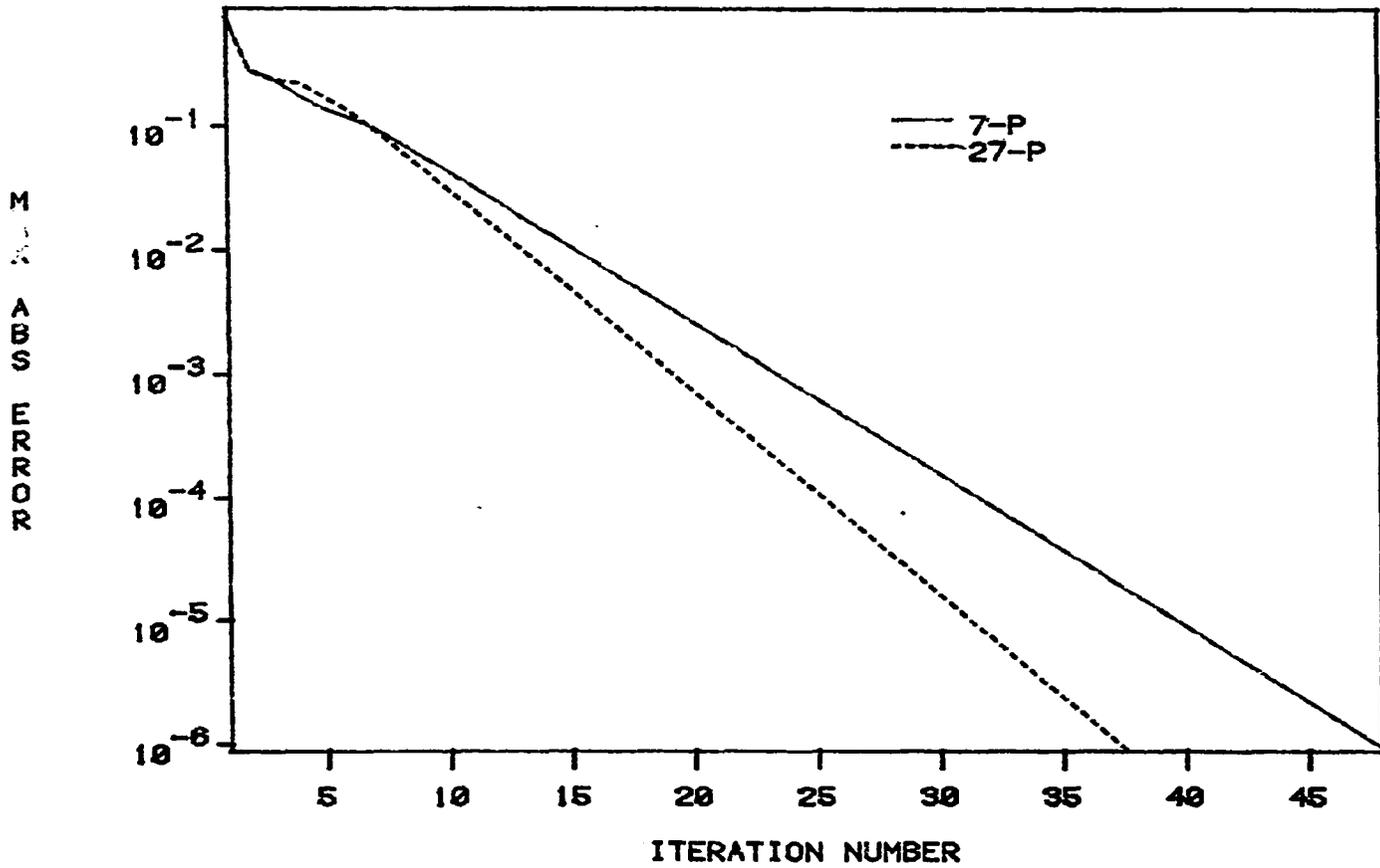


Figure 12. Maximum absolute error on ϕ for Dirichlet problem as a function of the number of iterations (step size of 0.16, $\lambda = 0.2$)

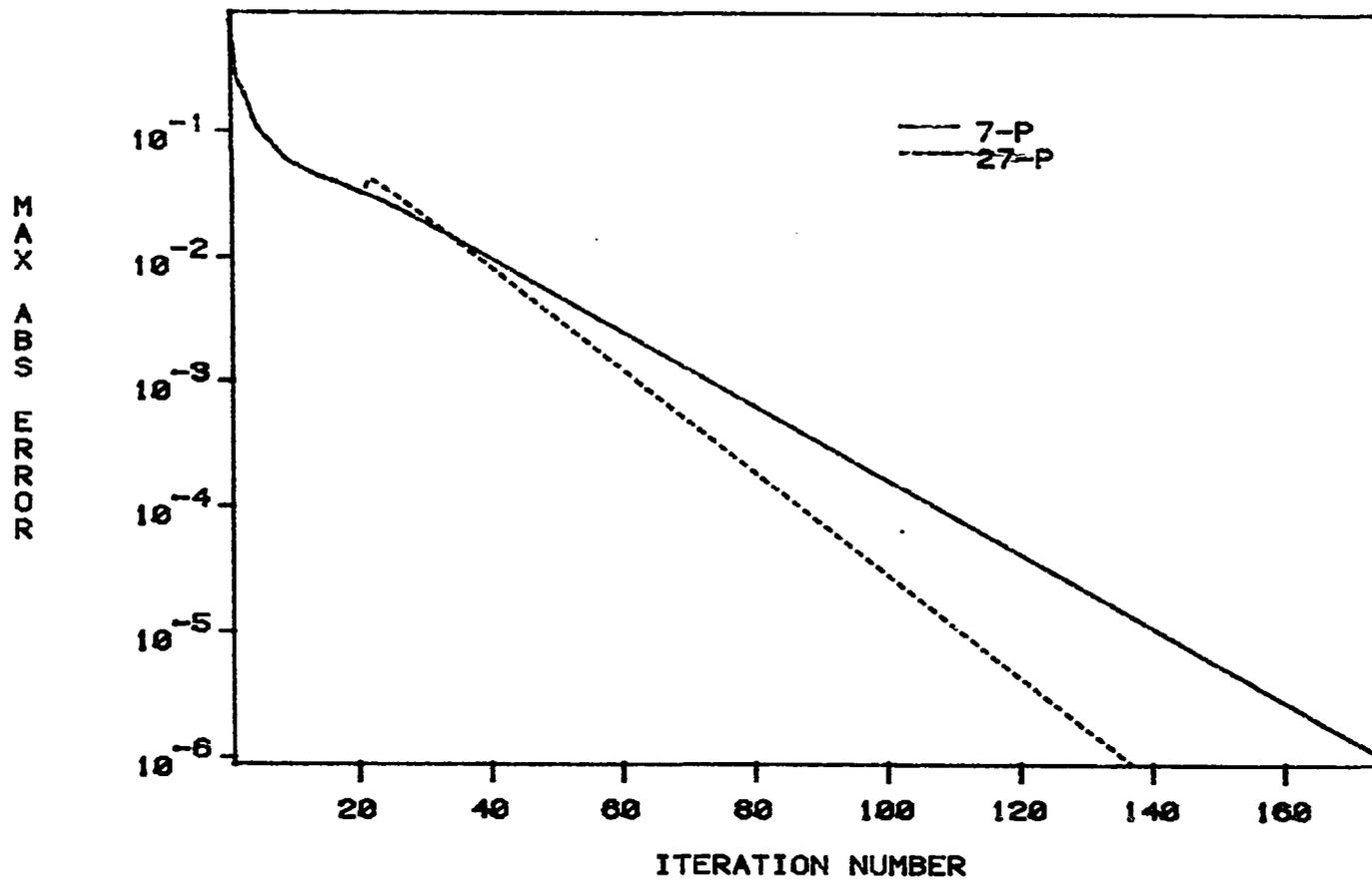


Figure 13. Maximum absolute error on ϕ for Dirichlet problem as a function of the number of iterations needed (step size of 0.08, $\lambda = 0.2$).

Table 5 lists the nodal flux values at the same locations for different step sizes. One can legitimately assume that the values corresponding to 13 nodes (1.029 to 3 S.D) might be considered sufficiently accurate to be taken as a standard to compare the other solutions against it. Then, one can observe that the final results given by the high order formula exhibit more stability. Moreover, with 4 nodes, the 27-point gives accurate results (to 3 S.D).

Table 5. Nodal flux values

Number of grids per side	4		7		13	
	7-point	27-point	7-point	27-point	7-point	27-point
Location 1	1.02533	1.02995	1.02837	1.02966	1.02928	1.02962
Location 2	1.02533	1.02995	1.02837	1.02967	1.02928	1.02962

Other types of problems (different boundary values, and symmetric boundaries with respect to the diagonal of the cube) are not shown here but have also been investigated. They all sustained the dominance of the 6th order approximation.

V.2.b. The boundary value problem established
from the analytical solution

As a final test to the model, the following boundary value problem was set up and solved. The equation to be solved is also equation 4; however, the boundary conditions are different. These are derived from the analytical solution. That is, equation 4 is solved with a free boundary for the entire domain. Then, for a portion of that domain, say the first octant, the same equation is solved, where this time, only the external sides of that sub-cube are set to zero. The other three sides are forced to the appropriate values of the analytical solution (see Figure 14).

In Tables 6a, 6b and 7 are registered the flux values at two locations for different mesh size and for different convergence criteria. In the first table, this criterion is 10^{-6} , while for the other two it is 10^{-8} .

An important observation is in order. It concerns the outputs of the 15-point and the 19-point methods. If one uses Table 6a, the 15-point, as already noticed before, converges faster than the 19-point formula. However, from Table 6b, no dissimilarities of any kind are perceptible.

This prompted the use of 10^{-8} for the relatively finer mesh results of Table 7. There, also, the 4th order models are very much alike.

In Figure 15, the logarithm of the absolute error of the nodal flux is plotted against the logarithm of the spacing. Here, again, the superiority of the 27-point model is clearly displayed. In fact,

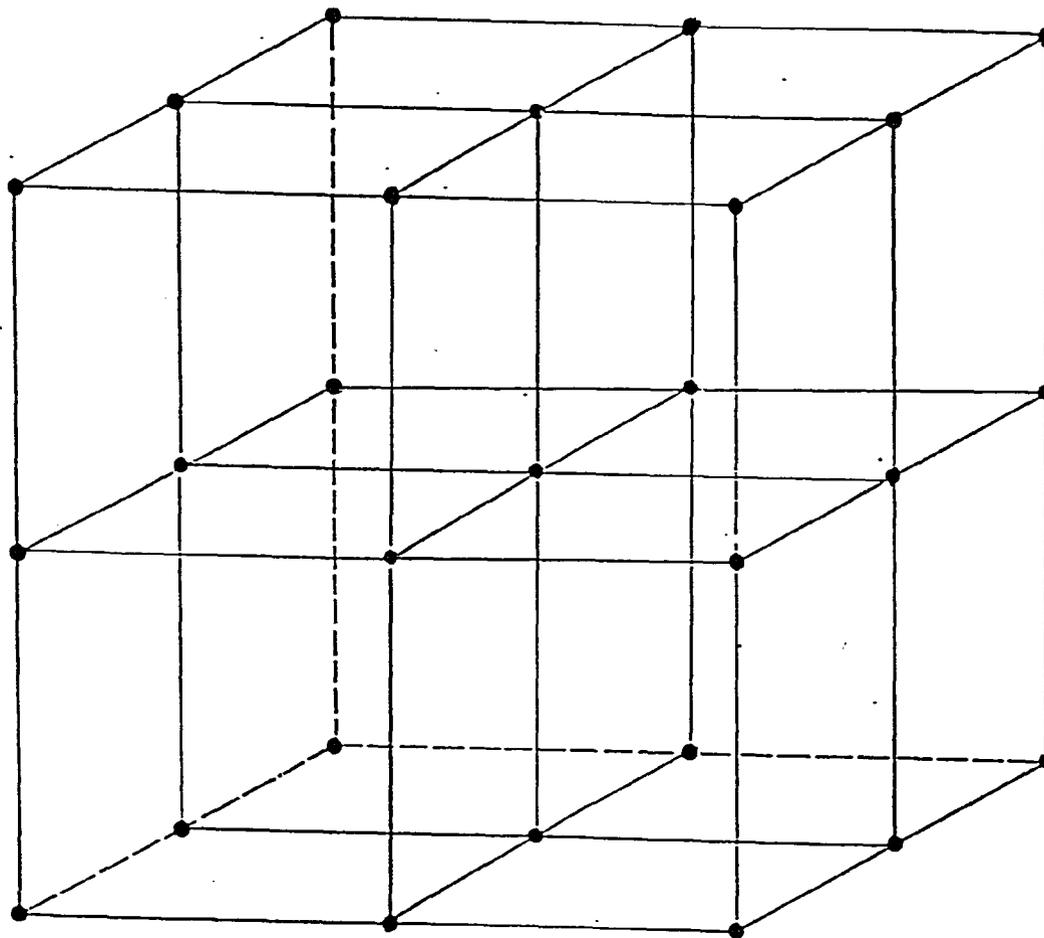


Figure 14. The sub-domain for which the boundary conditions are given by equation 58

Table 6a. Flux values at nodes 2 and 3 (convergence criterion 10^{-6})

Model	Iteration needed	Node 2			Node 3		
		Flux value	Absolute error	Relative error (%)	Flux value	Absolute error	Relative error (%)
Analytical		0.1249999	0.0		0.649519	0.0	
7-point	14	0.1267754	1.775484E-3	1.420	0.653605	4.086847E-3	0.630
15-point	14	0.1248758	1.241738E-4	0.099	0.649236	2.821057E-4	0.043
19-point	14	0.1247572	2.427130E-4	0.190	0.648972	4.086847E-3	0.043
27-point	13	0.1250122	1.222230E-5	0.009	0.649548	2.901271E-5	0.0045

Table 6b. Flux values at nodes 2 and 3 (convergence criterion 10^{-8})

Model	Iteration needed	Node 2			Node 3		
		Flux value	Absolute error	Relative error (%)	Flux value	Absolute error	Relative error (%)
Analytical		0.12499	0.0		0.649519	0.0	
7-point		0.12677	1.775826E-3	1.42	0.653605	4.086914E-3	0.630
15-point	18	0.12487	1.239001E-4	0.099	0.669236	2.820534E-4	0.043
19-point	19	0.12475	1.239001E-4	0.099	0.648972	2.820534E-4	0.043
27-point	17	0.12501	1.264506E-5	0.011	0.649548	2.909273E-5	0.0045

Table 7. Flux values at nodes 3 and 5 (convergence criterion 10^{-8})

Model	Iteration needed	Node 3			Node 5		
		Flux value	Absolute error	Relative error (%)	Flux value	Absolute error	Relative error (%)
Analytical		0.12499	0.0	0.0	0.649519	0.0	0.0
7-point	78	0.12546	4.641592E-4	0.37	0.650621	1.102101E-3	0.17
15-point	83	0.12499	7.712245E-7	0.006	0.649500	1.815782E-5	0.0028
19-point	86	0.12498	7.712245E-6	0.006	0.649485	1.815782E-5	0.0028
27-point	79	0.12500	1.611937E-7	0.00012	0.649519	4.422240E-7	0.00007

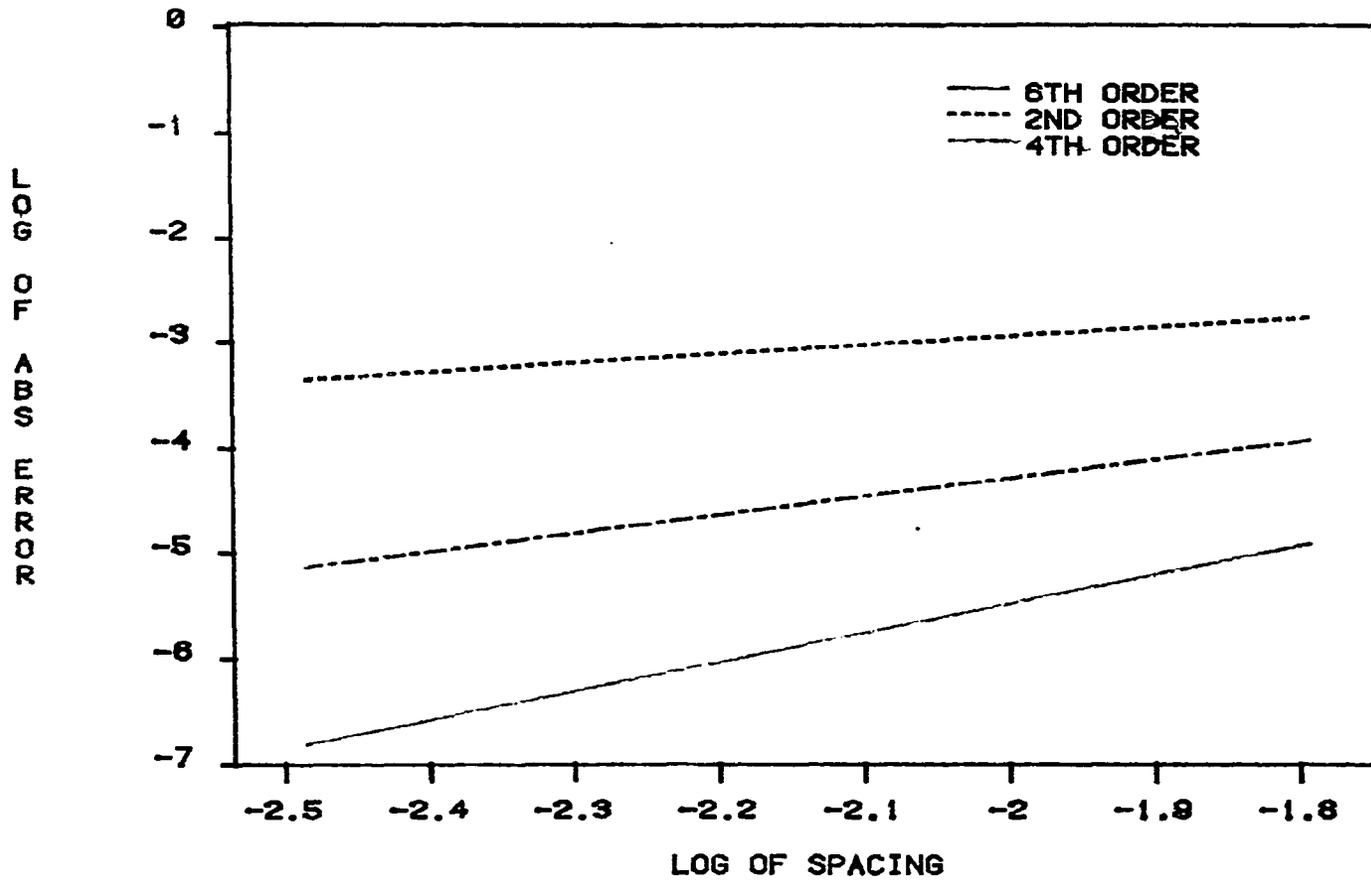


Figure 15. Log of maximum absolute error on ϕ as a function of the log of spacing for the sub-domain shown in Figure 14

for a given step size (H), the 6th order would generate similar or even better results than the 2nd order that uses just one-third of H.

V.3. Optimization

To provide an additional trial of the superiority (in accuracy and efficiency) of the 6th order approximation, the following types of optimization were attempted:

- i. Systems optimization;
- ii. SOR optimization; and
- iii. Vector processor optimization.

V.3.a. Systems optimization

All the previous problems were run on the VAX-VMS-11/780 system. From Table 1, one recalls that using the 27-point formula, the eigenvalue problem for 11 nodes converged in more than 2 minutes. Even though this is due to the severe convergence criterion (10^{-6}), one is still interested in reducing computational time.

Using the optimize option available on VAX, the execution time for this problem was reduced to 1 1/2 minutes. Moreover, the same problem was run on the NAS-AS/9160 in only 2 sec.

V.3.b. The SOR optimization

Hitherto only the particular value of one for the relaxation factor was used. However, to take advantage of the SOR use, an optimal value w_p of w should be determined. This is usually a tedious task.

For that reason, the usual trial and error technique will be applied to the 27-point formula for the problem mentioned in the foregoing paragraph.

Figure 16 shows the values of w versus the number of iterations needed for the same convergence criterion. One can observe that the optimal value for this problem is $w_p = 1.545$. Moreover, less than 36 sec was needed for convergence, as compared to 2 min, if $w = 1.0$.

V.3.c. The vector processor in optimization

As was stated at the beginning of this study, 3-D problems will be more and more attractive because of the availability of supercomputers. For this purpose, vector processing hardware available on the NAS computer was applied to the optimized version of the program which solved the eigenvalue problem cited above.

The FORTRAN source was preprocessed by the VAST (vector and array syntax translator) processor [50], to identify sections of the program which could take advantage of the VPF (vector processing facility).

Unexpectedly, the execution time was about 2.0 sec. In other words, the prognosticated savings in CPU time, from the VAST, were not attained. Table 8 lists the CPU times required by the different systems.

Table 8. CPU times to solve the eigenvalue problems using the 27-point relation on different computational systems

System	Vax Standard	Vax Optimized	NAS Scalar	NAS Vector
CPU (sec)	120	90	2	2

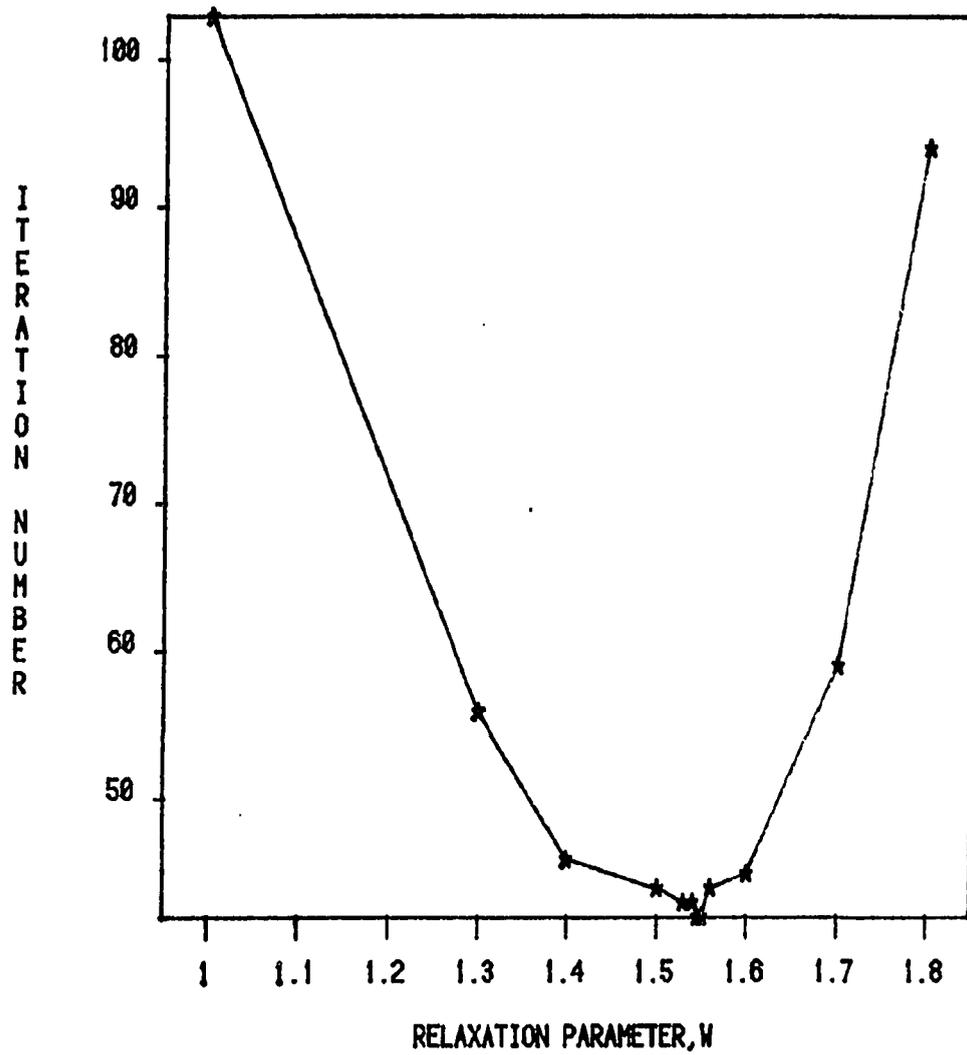


Figure 16. The number of iterations as a function of the SOR parameter w for the 27-point applied to the eigenvalue problem

According to J. Hoekstra [51], it was confirmed that the effectiveness of this processor is only significant for problems using loops (vector or arrays) of size 100 or greater.

The foregoing eigenvalue problem using 50 nodes per side was attempted. The CPU time needed was about 3 min. This is acceptable for the size of the problem and the rough vectorization which was made.

Furthermore, considering a fine mesh of this magnitude sounds inconsistent with the objective of this thesis. However, this is not so, because as was demonstrated by all the previous results, only the application of the 6th order approximation produces more accurate and efficient results, regardless of the step size.

Thus, to repeat, all of the above results support the feasibility and validity of the 27-point approximation.

VI. SUMMARY AND CONCLUSION

V.1. Summary

To demonstrate the advantages of using higher order F.D approximations in 3-D, the one group neutron diffusion equation has been solved for different reactor configurations. This corresponds to solving an eigenvalue or a boundary value problem. In applying the former, great savings (efficiency and memory) can be gained. In fact, the 27-point formula using 2 nodes performed better than the usual 7-point with 10 nodes (see Figure 5). This illustrates the memory savings, since with relatively larger mesh, for example, 3 times as large, one can achieve very accurate results (less 1%) if the 6th order model is utilized. Moreover, this precision is attained without any C.P.U. detriment (see Figure 6). Without any type of optimization (program and SOR optimization), the 2nd and 6th order converged in about 0.25 sec per node. This shows the efficiency of the 27-point formula.

For this class of problem, the determination of the eigenfunction has not clearly displayed the above-mentioned benefits of the 27-points. This prompted the study of other problems. For this purpose, two boundary value problems were analyzed. For the Dirichlet problem, the absence of the analytical solution required the use of a fine mesh (11x11x11) solution as a benchmark. The 27-point approximation converged faster (see Figures 10-13) than all the other models. However, the solutions can be considered as comparable (to the 3rd S.D). In spite of that, for the smaller step sizes (see Table 5), the high order

approximation gave accurate results (to the 3rd S.D.).

To satisfy the desire to establish the model and as a final test to its credibility, the analytical-boundary value problem was considered. The flux values at the same locations for different step sizes and convergence criteria are found in Tables 6-7. The absolute errors in terms of the spacings are in Figure 15. As anticipated, all these results display once more the absolute performances of the higher order approximations.

V.2. Conclusions

Considerable (up to 94%) computational savings can be accomplished in three-dimensional calculations using the 6th order (27-point relations) or even the 4th order (15- or 19-point relations) rather than the 2nd order (usual 7-point relations) model. To demonstrate these facts, the one group neutron diffusion equation was solved for different reactor problems.

The availability of the analytical solution for the free boundary reactor permitted its use as a benchmark to compare to the numerical calculations of either the eigenvalue or the eigenfunctions. For the B^2 calculations, the use of 6 nodes per side with the 27-point relation would have been more than enough for numerous practical situations, since the maximum relative error is only 0.043%. To obtain similar results, the 7-point relation should require more than 20 nodes per side. Moreover, the analytical solution played a great role in establishing the credibility of the higher order models. In that way, it was confirmed

that the use of numerical approximations to the 4th and 6th order mixed operators has no effect on the efficiency of the overall calculations.

Furthermore, the effectiveness in the flux computations was displayed through the solution of non-vacuum boundary problems. For the case where the fine mesh was used as the benchmark, it was concluded that the 6th order approximation using 4 nodes per side generated very accurate results. This is translated in memory savings of more than 90%. In the same manner, for the analytical boundary value problem, the 27-point formula reduced the error to less than 0.0045% when it used 7 nodes, as compared to the 7-point relation which decreased it to only 0.63%.

Finally, the different types of optimization substantiated, once more, the great advantages when using the 27-point relation. In that respect, the use of the optimal relaxation parameter w_p reduced considerably (70%) the time and the number of iterations needed for convergence. In addition to that, the use of optimized versions of the VAX or the NAS can result in significant decreases in CPU times.

In conclusion, all the investigated problems illustrated clearly the ultimate superiority of the 27-point approximation.

VII. SUGGESTIONS FOR FURTHER STUDIES

1. The natural extension of this model is the application of the general mixed boundary condition or albedo condition of the form:

$$\alpha \frac{\partial \phi}{\partial n} + \tau \phi + \kappa \equiv 0 \quad (1)$$

where α , τ and κ are constants and $\partial/\partial n$ is the normal derivative.

Condition 1 can only be used if one uses a numerical approximation to the first derivative. Usually, a central divided difference is used. However, for consistency with our model, the $\partial/\partial n$ should also be approximated using a higher order expansion. The procedure will be similar to that of Chapter II. Work on this problem has been started.

2. The other important suggestion is to apply the model to a system of equations, each containing the Laplacian. This will be of interest to the multigroup neutron diffusion equation.
3. The development of the fundamental equation for nonequal spacings, either rectangular or curvilinear, will be of interest. For this purpose, some developments are also underway.
4. The straightforward incorporation of this model to existing finite difference packages using uniform cubic spacing will be a valuable contribution to their improvement.
5. The use of this method in a hybrid model has been considered where a fine mesh calculation can be performed on a unit node of a nodal method. The connection between the two models will be through the

function and its 1st derivative (flux and current) at the unit node interfaces.

6. Finally, this model can be perfected by using some accelerating techniques to the SOR, or by applying a Fast Fourier analysis [30]. In this case, the difference equations, obtained after applying the boundary conditions:

$$\Gamma U = b$$

are solved using a combination of a cyclic reduction and Fourier Analysis. The method should result in even reduced execution time [43].

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IX. ACKNOWLEDGMENTS

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X. APPENDIX A. TAYLOR EXPANSION

We exhibit the Taylor expansion of the terms of equation 15 about the central node (i,j,k) . Using equation 30, the expansion along the 3 positive directions, i.e., $i+1$, $j+1$ and $k+1$, yields

$$\begin{aligned} \phi_{i+1,j+1,k+1} = & [1 + (\delta + \eta + \xi) + \frac{1}{2!}(\delta + \eta + \xi)^2 + \\ & \frac{1}{3!}(\delta + \eta + \xi)^3 + \frac{1}{4!}(\delta + \eta + \xi)^4 + \frac{1}{5!}(\delta + \eta + \xi)^5 + \\ & \frac{1}{6!}(\delta + \eta + \xi)^6 + \frac{1}{7!}(\delta + \eta + \xi)^7 + O(h^8)] \phi_0 \end{aligned} \quad (X-1)$$

Similarly, along positive (i,j) and negative k , i.e., $(i+1, j+1, k-1)$, one gets:

$$\begin{aligned} \phi_{i+1,j+1,k-1} = & [1 + (\delta + \eta - \xi) + \frac{1}{2!}(\delta + \eta - \xi)^2 + \\ & \frac{1}{3!}(\delta + \eta - \xi)^3 + \frac{1}{4!}(\delta + \eta - \xi)^4 + \frac{1}{5!}(\delta + \eta - \xi)^5 + \\ & \frac{1}{6!}(\delta + \eta - \xi)^6 + \frac{1}{7!}(\delta + \eta - \xi)^7 + O(h^8)] \phi_0 \end{aligned} \quad (X-2)$$

Then, along the positive (i,k) and negative j , i.e., $(i+1, j-1, k+1)$, one finds:

$$\begin{aligned} \phi_{i+1,j-1,k+1} = & [1 + (\delta - \eta + \xi) + \frac{1}{2!}(\delta - \eta + \xi)^2 + \\ & \frac{1}{3!}(\delta - \eta + \xi)^3 + \frac{1}{4!}(\delta - \eta + \xi)^4 + \frac{1}{5!}(\delta - \eta + \xi)^5 + \\ & \frac{1}{6!}(\delta - \eta + \xi)^6 + \frac{1}{7!}(\delta - \eta + \xi)^7 + O(h^8)] \phi_0 \end{aligned} \quad (X-3)$$

and finally, for the positive (j,k) and negative i , i.e., $(i-1, j-1, k+1)$,

one gets:

$$\begin{aligned} \phi_{i-1,j+1,k+1} &= [1 + (-\delta + \eta + \xi) + \frac{1}{2!}(-\delta + \eta + \xi) + \\ &\frac{1}{3!}(-\delta + \eta + \xi)^3 + \frac{1}{4!}(-\delta + \eta + \xi)^4 + \frac{1}{5!}(-\delta + \eta + \xi)^5 + \\ &\frac{1}{6!}(-\delta + \eta + \xi)^6 + \frac{1}{7!}(-\delta + \eta + \xi)^6 + O(h^8)]\phi_0 \end{aligned} \quad (X-4)$$

On the other hand, the expansions along the three negative directions, i.e., $i-1$, $j-1$, and $k-1$, give:

$$\begin{aligned} \phi_{i-1,j-1,k-1} &= [1 + (-\delta - \eta - \xi) + \frac{1}{2!}(-\delta - \eta - \xi)^2 + \\ &\frac{1}{3!}(-\delta - \eta - \xi)^3 + \frac{1}{4!}(-\delta - \eta - \xi)^4 + \frac{1}{5!}(-\delta - \eta - \xi)^5 + \\ &\frac{1}{7!}(-\delta - \eta - \xi)^6 + \frac{1}{7!}(-\delta - \eta - \xi)^7 + O(h^8)]\phi_0 \end{aligned} \quad (X-5)$$

Then, for the negative (i,j) and positive k , i.e., $i-1$, $j-1$, $k+1$, one gets:

$$\begin{aligned} \phi_{i-1,j-1,k+1} &= [1 + (-\delta - \eta + \xi) + \frac{1}{2!}(-\delta - \eta + \xi)^2 + \\ &\frac{1}{3!}(-\delta - \eta + \xi)^3 + \frac{1}{4!}(-\delta - \eta + \xi)^4 + \frac{1}{5!}(-\delta - \eta + \xi)^5 + \\ &\frac{1}{6!}(-\delta - \eta + \xi)^6 + \frac{1}{7!}(-\delta - \eta + \xi)^7 + O(h^8)]\phi_0 \end{aligned} \quad (X-6)$$

Similarly, for the negative (i,k) and positive j , i.e., $i-1$, $j+1$ and $k-1$, one obtains:

$$\begin{aligned} \phi_{i-1,j+1,k-1} &= [1 + (-\delta + \eta - \xi) + \frac{1}{2!}(-\delta + \eta - \xi)^2 + \\ &\frac{1}{3!}(-\delta + \eta - \xi)^3 + \frac{1}{4!}(-\delta + \eta - \xi)^4 + \frac{1}{5!}(-\delta + \eta - \xi)^5 + \\ &\frac{1}{6!}(-\delta + \eta - \xi)^6 + \frac{1}{7!}(-\delta + \eta - \xi)^7 + O(h^8)]\phi_0 \end{aligned} \quad (X-7)$$

Finally, the expansion along the negative (j,k) and positive i, i.e., i+1, j-1 and k-1, yields:

$$\begin{aligned} \phi_{i+1,j-1,k-1} = & [1 + (\delta - \eta - \xi) + \frac{1}{2!}(\delta - \eta - \xi)^2 + \\ & \frac{1}{3!}(\delta - \eta - \xi)^3 + \frac{1}{4!}(\delta - \eta - \xi)^4 + \frac{1}{5!}(\delta - \eta - \xi)^5 + \\ & \frac{1}{6!}(\delta - \eta - \xi)^6 + \frac{1}{7!}(\delta - \eta - \xi)^7 + O(h^8)]\phi_0 \end{aligned} \quad (X-8)$$

Equations X-1 to X-8 are substituted back into equation 15. The resulting equation will only be written after it is simplified. A good way to reduce it is to use the values of n, which are the powers of the quantity $(\pm\delta \pm \eta \pm \xi)^n \phi_0$.

Case 1: n=0, this corresponds to the first term of each of the above equations. Therefore, summing will yield:

$$8 \phi_0 \quad (X-9)$$

Case 2: n=1, this corresponds to the 2nd term; i.e., terms with $(\pm\delta \pm \eta \pm \xi)$. It is easy to find that the sum of these terms results in zero.

Case 3: n=2, this is the 3rd term in each of the above equations. Here, one uses the elementary identity, i.e., $(\pm a \pm b \pm c)^2$, to discover, after development, that all the mixed terms cancel one another; thereupon, one gets:

$$8(\delta^2 + \eta^2 + \xi^2)\phi_0 \quad (X-10)$$

Case 4: $n=3$, this is the 4th term in the equations. Again, using the identity $(\pm a \pm b \pm c)^3$, one perceives also that the sum of the resulting terms is zero. Furthermore, for $n=5$ and $n=7$, no contributions are expected.

Case 5: $n=4$, this is the 5th term. This time, one uses the relation $(\pm a \pm b \pm c)^4$. As for case 3, all the mixed terms with odd power cancel one another. The only quantities left from the sum will be:

$$8[(\delta^4 + \eta^4 + \xi^4) + 6(\delta^2\eta^2 + \delta^2\xi^2 + \eta^2\xi^2)]\phi_0 \quad (X-11)$$

Case 6: $n=6$, this is the last term considered in equations X-1 to X-8. Using the identity $(\pm a \pm b \pm c)^6$, all the terms, up to the 6th power, will drop off except the following:

$$\begin{aligned} & \left[\frac{1}{6!}(\delta^6 + \eta^6 + \xi^6) + \frac{15}{6!}[\delta^2(\eta^4 + \xi^4) + \eta^2(\delta^4 + \xi^4) \right. \\ & \left. + \xi^2(\delta^4 + \eta^4)] + \frac{90}{6!}\delta^2\eta^2\xi^2 \right] \phi_0 \end{aligned} \quad (X-12)$$

Finally, using equations X-9 to X-12, equation 15 becomes:

$$\begin{aligned} \phi_C = & 8\left[1 + \frac{1}{2!}(\delta^2 + \eta^2 + \xi^2) + \frac{1}{4!}(\delta^4 + \eta^4 + \xi^4) + \right. \\ & \frac{6}{4!}(\delta^2\eta^2 + \delta^2\xi^2 + \eta^2\xi^2) + \frac{1}{6!}(\delta^6 + \eta^6 + \xi^6) + \\ & \frac{15}{6!}[\delta^2(\eta^4 + \xi^4) + \eta^2(\delta^4 + \xi^4) + \xi^2(\delta^4 + \eta^4) + \\ & \left. \frac{90}{6!}\delta^2\eta^2\xi^2] \phi_0 + O(h^8) \end{aligned} \quad (X-13)$$

XI. APPENDIX B. NUMERICAL EVALUATION OF THE 4TH ORDER MIXED OPERATOR

This term will be obtained by the appropriate combination of the expansions 20, 29 and 31, rewritten here:

$$\phi_N \equiv 2\left[3 + \frac{h^2}{2!}(\nabla^2) + \frac{1}{4!}(\delta^4 + \eta^4 + \xi^4)\right] \delta_0 + O(h^8) \quad (\text{XI-1})$$

$$\begin{aligned} \phi_E \equiv & 4\left[3 + \frac{2}{2!}(\nabla^2) + \frac{2}{4!}(\delta^4 + \eta^4 + \xi^4) + \right. \\ & \left. \frac{6}{4!}(\delta^2\eta^2 + \delta^2\xi^2 + \eta^2\xi^2) + \frac{2}{6!}(\delta^6 + \eta^6 + \xi^6) + \right. \\ & \left. \frac{15}{6!}(\delta^4\eta^2 + \delta^4\xi^2 + \eta^4\xi^2 + \eta^4\delta^2 + \xi^4\delta^2 + \xi^4\eta^2)\right] \phi_0 + O(h^8) \quad (\text{XI-2}) \end{aligned}$$

$$\begin{aligned} \phi_C \equiv & 8\left[1 + \frac{h^2}{2!}(\nabla^2) + \frac{1}{4!}(\delta^4 + \eta^4 + \xi^4) + \right. \\ & \left. \frac{6}{4!}(\delta^2\eta^2 + \delta^2\xi^2 + \eta^2\xi^2) + \frac{1}{6!}(\delta^6 + \eta^6 + \xi^6) + \right. \\ & \left. \frac{15}{6!}(\delta^4\eta^2 + \delta^4\xi^2 + \eta^4\delta^2 + \eta^4\xi^2 + \eta^4\delta^2 + \xi^4\eta^2) + \right. \\ & \left. \frac{90}{6!}(\delta^2\eta^2\xi^2 + \dots)\right] \phi_0 + O(h^8) \quad (\text{XI-3}) \end{aligned}$$

since $(D^2)_{ij} \equiv (D_{xy}^2 + D_{xz}^2 + D_{yz}^2)$

or

$$(D^2)_{ij} \equiv \frac{1}{h^4}(\delta^2\eta^2 + \delta^2\xi^2 + \eta^2\xi^2) \quad (\text{XI-4})$$

Therefore, to derive it from equations XI-1 to XI-3, one needs to end these approximations at the 6th order at least.

If one effectuates the difference:

$$\phi_C - \phi_E$$

all the terms will cancel one another, except the following:

$$8\phi_o + \frac{8 \times 6}{4!}(\delta^2 \eta^2 + \delta^2 \xi^2 + \eta^2 \xi^2) - 12\phi_o - \frac{4 \times 6}{4!}(\delta^2 \eta^2 + \delta^2 \xi^2 + \eta^2 \xi^2) \quad (\text{XI-5})$$

which yields:

$$\phi_C - \phi_E \equiv (\delta^2 \eta^2 + \delta^2 \xi^2 + \eta^2 \xi^2) - 4\phi_o + 0(h^6)$$

or

$$(\delta^2 \eta^2 + \delta^2 \xi^2 + \eta^2 \xi^2) \equiv \phi_C - \phi_E + 4\phi_o + 0(h^6) \quad (\text{XI-6})$$

Using equation B-4, there results:

$$(D^2)_{ij} \phi_o \equiv \frac{1}{h^4}(\phi_C - \phi_E + 4\phi_o) + 0(h^2) \quad (\text{XI-7})$$

Still, another combination of equations (XI-1 to XI-3) may permit the evaluation of $(D^2)_{ij} \phi_o$. For this, one considers the following:

$$\phi_E - 4\phi_N$$

which gives:

$$\phi_E - 4\phi_N \equiv -12\phi_o + (\delta^2 \eta^2 + \delta^2 \xi^2 + \eta^2 \xi^2) + 0(h^6)$$

or

$$(D^2)_{ij} \phi_o \equiv \frac{1}{h^4}(\phi_E - 4\phi_N + 12\phi_o) + 0(h^2) \quad (\text{XI-8})$$

At this point, two approximations for the operator $(D^2)_{ij}$ are available. Both are 2nd order. The only difference between them is that in equation XI-7, 20 evaluations (8 corners and 12 edges) are required, whereas in equation XI-8, 18 evaluations (12 edges and 6 faces)

are needed. In considering the number of iterations and the work needed, approximation XI-8 will be selected.

XII. APPENDIX C. DETERMINATION OF p AND p' TO
OBTAIN THE 6TH ORDER TRUNCATION ERROR

One needs to solve the system (44) (48) rewritten here:

$$\nabla^4 + (-2 + 3p + 6p')(D^2)_{ij}\phi_o \equiv 0 \quad (\text{XII-1})$$

$$\nabla^6 + (-3 + \frac{15}{2}p + 15p')\nabla^2(D^2)_{ij}\phi_o + (3 - \frac{45}{2}p')D_{xyz}^2\phi_o \equiv 0 \quad (\text{XII-2})$$

Equation XII-1 can also be written as follows:

$$[\nabla^4 - 2(D^2)_{ij} + 3p(D^2)_{ij} + 6p'(D^2)_{ij}]\phi_o \equiv 0 \quad (\text{XII-3})$$

from which one gets:

$$p \equiv \frac{[2(D^2)_{ij} - \nabla^4 - 6p'(D^2)_{ij}]\phi_o}{3(D^2)_{ij}\phi_o}$$

or

$$p = \frac{2}{3} - \frac{1}{3} \frac{\nabla^4\phi_o}{(D^2)_{ij}\phi_o} - 2p' \quad (\text{XII-4})$$

Equation XII-2 can then be written as:

$$\begin{aligned} \nabla^6 - 3\nabla^2(D^2)_{ij} + \frac{15}{2}p\nabla^2(D^2)_{ij} + 15p'\nabla^2(D^2)_{ij} \\ + 3D_{xyz}^2 - \frac{45}{2}pD_{xyz}^2 + 45p'D_{xyz}^2 \equiv 0 \end{aligned} \quad (\text{XII-5})$$

or

$$\begin{aligned} \nabla^6 - 3\nabla^2(D^2)_{ij} + 3D_{xyz}^2 + \frac{15}{2}p[\nabla^2(D^2)_{ij} - 3D_{xyz}^2] + \\ + 15p'[\nabla^2(D^2)_{ij} + 3D_{xyz}^2] \equiv 0 \end{aligned} \quad (\text{XII-6})$$

Now, equation XII-4 is plugged into equation XII-6:

$$\begin{aligned} & \nabla^6 - 3\nabla^2(D^2)_{ij} + 3D_{xyz}^2 + 15 p' [\nabla^2(D^2)_{ij} + 3D_{xyz}^2] \\ & + \frac{15}{2} \left[\left(\frac{2}{3} - \frac{1}{3} \frac{\nabla^4}{(D^2)_{ij}} - 2p' \right) (\nabla^2(D^2)_{ij} - 3D_{xyz}^2) \right] = 0 \end{aligned} \quad (\text{XII-7})$$

or

$$90 D_{xyz}^2 p' - \frac{3}{2} \nabla^6 - 12 D_{xyz}^2 + 2\nabla^2(D^2)_{ij} + \frac{15}{2} \frac{\nabla^4 D_{xyz}^2}{(D^2)_{ij}} = 0$$

From which,

$$p' = \frac{1/2 [3\nabla^6 + 24 D_{xyz}^2 - 4\nabla^2(D^2)_{ij} - 15 \frac{\nabla^4 D_{xyz}^2}{(D^2)_{ij}}]}{90 D_{xyz}^2}$$

or

$$p' = \frac{2}{15} + \frac{1}{2} \left[\frac{1}{90 D_{xyz}^2} (3\nabla^6 - 4\nabla^2(D^2)_{ij}) - \frac{1}{6} \frac{\nabla^4}{(D^2)_{ij}} \right] \quad (\text{XII-8})$$

If we let,

$$B = \frac{1}{6} \frac{\nabla^4 \phi_0}{(D^2)_{ij} \phi_0} \quad (\text{XII-9})$$

and

$$A = \frac{1}{90 (D_{xyz}^2) \phi_0} [-3\nabla^6 + 4\nabla^2(D^2)_{ij}] \phi_0 \quad (\text{XII-10})$$

so that equation XII-8 becomes:

$$p' = \frac{2}{15} + \frac{1}{2} (A - B) \quad (\text{XII-11})$$

Now, if equation XII-11 is substituted in equation XII-4, and using equations XII-9 and XII-10, we get:

$$P = \frac{2}{5} - \frac{1}{3} \frac{\nabla^4}{(D^2)_{ij}} - A + B \quad (\text{XII-12})$$

$$P = \frac{2}{5} - (A + B) \quad (\text{XII-13})$$

XIII. APPENDIX D. NUMERICAL EVALUATION OF THE 6TH ORDER MIXED OPERATOR

One recalls from equation 46 that:

$$(D^2)_{xyz} \phi_o = \frac{1}{h^6} \delta^2 \eta^6 \xi^2 \quad (\text{XIII-1})$$

Therefore, to obtain this operator, the expansions XI-1 to XI-3 will be considered as shown because their T.E is $O(h^8)$.

Consider:

$$\phi_C - 2\phi_E + 4\phi_N$$

Substituting the corresponding expansion, all the terms will cancel except:

$$8 \phi_o + \frac{8 \times 90}{6!} \delta^2 \eta^2 \xi^2 \phi_o \quad (\text{XIII-2})$$

which, when using equation XIII-1, results in:

$$(D^2)_{xyz} \phi_o = \frac{1}{h^6} (\phi_C - 2\phi_E + 4\phi_N - 8\phi_o) + O(h^2) \quad (\text{XIII-3})$$

In contrast with the evaluation of the 4th order operator $(D^2)_{ij}$, expression XIII-3 is a unique expression for the 6th order operator $(D^2)_{xyz}$.

XIV. APPENDIX E. EVALUATION OF THE MIXED OPERATORS,
 p AND p' FROM THE ANALYTICAL SOLUTION

Recall that the analytical solution is given by:

$$\phi(x,y,z) = \sin \alpha x \sin \alpha y \sin \alpha z \quad (\text{XIV-1})$$

where:

$$\alpha = \pi/L_x \text{ and}$$

$$L_x = 1.$$

XIV.1. Evaluation of the 4th Order Mixed Operator

From equation 38:

$$(D^2)_{ij} \equiv (D_{xy}^4 + D_{yz}^4 + D_{zx}^4) \quad (\text{XIV-2})$$

where:

$$D_{xy}^4 \equiv \frac{\partial^2}{\partial x^2} \left(\frac{\partial^2}{\partial y^2} \right) \quad (\text{XIV-3})$$

$$D_{yz}^4 \equiv \frac{\partial^2}{\partial y^2} \left(\frac{\partial^2}{\partial z^2} \right) \quad (\text{XIV-4})$$

$$D_{zx}^4 \equiv \frac{\partial^2}{\partial z^2} \left(\frac{\partial^2}{\partial x^2} \right) \quad (\text{XIV-5})$$

Using equation XIV-1 in XIV-3 yields:

$$D_{xy}^4 \phi = \frac{\partial^2}{\partial x^2} (-\alpha^2 \phi)$$

$$D_{xy}^4 \phi = \alpha^4 \phi \quad (\text{XIV-6})$$

Similarly, the use of equation XIV-1 in XIV-4 and XIV-5 yields:

$$D_{yz}^4 = \alpha^4 \phi \quad (\text{XIV-7})$$

and

$$D_{zx}^4 = \alpha^4 \phi \quad (\text{XIV-8})$$

Therefore, equation XIV-2 becomes:

$$(D^2)_{ij} = 3\alpha^4 \phi \quad (\text{XIV-9})$$

XIV.2. Evaluation of the 6th Order Mixed Operator

From equation 46,

$$(D^2)_{xyz} \phi \equiv \left(\frac{\partial^2}{\partial x^2} \left(\frac{\partial^2}{\partial y^2} \left(\frac{\partial^2}{\partial z^2} \phi \right) \right) \right) \quad (\text{XIV-10})$$

Using equation XIV-1,

$$\frac{\partial^2}{\partial z^2} = -\alpha^2 \phi \quad (\text{XIV-11})$$

Therefore,

$$\frac{\partial^2}{\partial y^2} \left(\frac{\partial^2}{\partial z^2} \phi \right) = \alpha^4 \phi \quad (\text{XIV-12})$$

Finally,

$$\frac{\partial^2}{\partial x^2} \left(\frac{\partial^2}{\partial y^2} \left(\frac{\partial^2}{\partial z^2} \phi \right) \right) = -\alpha^6 \phi \quad (\text{XIV-13})$$

so that equation XIV-10 yields:

$$(D^2)_{xyz} \phi = -\alpha^6 \phi \quad (\text{XIV-14})$$

XIV.3. Evaluation of p and p' for the 4th Order Truncation Error

Equation 41 gives:

$$p = \frac{2}{3} - \frac{\nabla^4 \phi}{3(D^2)_{ij} \phi} \quad (\text{XIV-15})$$

Since,

$$\nabla^2 \phi = -B^2 \phi$$

Then,

$$\nabla^4 \phi = B^4 \phi \quad (\text{XIV-16})$$

Finally, using equations XIV-9 and XIV-16 in XIV-15, one gets:

$$p = \frac{2}{3} - \frac{B^4 \phi}{6\alpha^4 \phi}$$

or

$$p = \frac{2}{3} - \frac{B^4}{6\alpha^4} \quad (\text{XIV-17})$$

Similarly, using equation 47:

$$p' = \frac{1}{3} - \frac{B^4}{18\alpha^4} \quad (\text{XIV-18})$$

XIV.4. Evaluation of p and p' for the 6th Order Truncation Error

For this purpose, one needs to evaluate the quantities A and B .

Using equations XII-9 and XII-10:

$$B = \frac{1}{6} \frac{\nabla^4 \phi}{(D^2)_{ij} \phi} \quad (\text{XIV-19})$$

$$A = \frac{1}{90(D_{xyz}^2)_\phi} [-3v^6 + 4v^2(D^2)_{ij}]_\phi \quad (\text{XIV-20})$$

Using equations XIV-9 and XIV-16, equation XIV-19 becomes:

$$B = \frac{1}{18} \frac{B^4}{\alpha^4} \quad (\text{XIV-21})$$

and equation XIV-20 yields:

$$A \equiv \frac{1}{90(-\alpha^6)_\phi} [3B^6_\phi - 4B^2 (3\alpha^4)_\phi]$$

or

$$A = \frac{-1}{90\alpha^6} [3B^6 - 12 B^2 \alpha^4] \quad (\text{XIV-22})$$