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FINITE DIFFERENCE METHOD FOR SOLVING THE SPATIO-TEMPORAL DIFFUSION EQUATION IN THE TWO-GROUP APPROXIMATION

COMPARISON BETWEEN THE SOLUTION BY AN ITERATIVE AND A DIRECT METHOD

by

R. MONTEROSSO and E. VINCENTI

1964

Joint Nuclear Research Center
Ispra Establishment - Italy

Reactor Physics Department and
Scientific Data Processing Center - CETIS

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CONTENTS

Preface

This report describes a part of a numerical program made for the study of the spatio-temporal dynamics of a reactor. The time-dependent two-group diffusion equations are transformed, by the finite difference method, into a system of linear equations.

This program was written for the Reactor TESI which operates in condition of prompt criticality and has fluxes which increase very rapidly. High accuracy is therefore required in calculating the fluxes at every time step. For this reason the solution of the system of linear equations was attempted in two ways, by an iterative method, as it is common practice in the nuclear codes, and by a direct method.

This report describes only the two methods used and gives a comparison of their numerical results. A complete description of the program and of the physical problem will be the subject of another report.

We are indebted to Dr. Guerri and Dr. Galligani for many useful suggestions.

I. The finite-difference formulation of the diffusion equations

In this report are described two mathematical methods to be employed in a program for the study of the spatio-temporal reactor dynamics. In this program the time dependent diffusion equations are solved directly with a numerical method in order to study the variations of the neutronic flux as a function of space and time throughout the core.

This problem is treated in the two-group approximation in order to better evaluate the flux distribution in the reflectors and their influence on the neutron economy.

For simplicity the reactor is imagined as an infinite horizontal slab of finite height H. Along the z-axis the reactor consists of several regions R_k of different physical nature: lower reflector, non rodded core, rodded core, upper reflector.

The two-group diffusion equations of the k-th region R_k are the following:

$$D_f^k \frac{\partial^2}{\partial z^2} \psi - A^k \psi + B^k \varphi + C^k = \frac{1}{w^k} \frac{\partial \psi}{\partial t} \qquad (1\text{-I})$$

$$D_t^k \frac{\partial^2}{\partial z^2} \varphi - E^k \varphi + F^k \psi = \frac{1}{v^k} \frac{\partial \varphi}{\partial t} \qquad (2\text{-I})$$

where:

D_f^k and D_t^k are the fast and thermal diffusion coefficients, which are assumed to be constant in each region R_k.

$\psi = \psi(z,t)$ = fast flux

$\varphi = \varphi(z,r)$ = thermal flux

$A^k = \left[\Sigma_R(z,t) + B^2 . D_f^k \right]$ = removal X-section and fast radial leakage.

$B^k = (1 - \beta) \cdot \nu \cdot \Sigma_f(z,t)$ = prompt neutrons produced per unity of thermal flux

$C^k = \lambda \cdot C\ (z,t)$ = delayed neutrons produced per cm^3 per sec.

$E^k = \left[\Sigma_a(z,t) + \Sigma_p(z,t) + B^2 \cdot D_t^k \right]$ = thermal absorption X-section, rod poison, thermal radial leakage

$F^k = \Sigma_R(z,t)$ = number of neutrons thermalized per unity of fast flux

w^k = neutron velocity of the fast group

v^k = neutron velocity of the thermal group

The quantities with index k are assumed to be continuous in each region R_k and may be discontinuous at the interfaces.

The fluxes ψ and φ and the neutron currents $D_f \frac{\partial \psi}{\partial z}$; $D_t \frac{\partial \varphi}{\partial z}$ are continuous functions everywhere.

The fluxes ψ and φ are zero at the lower and upper boundary of the reactor:

$$\varphi\ (0,t) = \varphi\ (H,t) = \psi\ (0,t) = \psi\ (H,t) = 0$$

The height of the reactor has been divided into mesh-points $\{z_l\}$ $(i = 0, 1, 2, \ldots.L, L+1)$ with $z_o = 0$; $z_{L+1} = H$. On each interface between two regions is a point of the lattice, and each region contains at least one point.

Discretizing also the time-variable t the diffusion equations (1-I) and (2-I) are transformed into:

$$-r_{l1} \cdot \psi_{l-1}^n + p_{l1} \cdot \psi_l^n - r_{l+1,1} \cdot \psi_{l+1}^n - s_l \cdot \varphi_l = q_{l1} \qquad (3\text{-I})$$

$$-m_i \cdot \psi_{i-1}^{n} - r_{i2} \cdot \varphi_{i-1}^{n} + p_{i2} \cdot \varphi_i^{n} - r_{i+1,2} \cdot \varphi_{i+1} = q_{i\ 2} \qquad (4\text{-I})$$

$(i = 1, 2, \ldots\ldots, L)$ space index

$(n = 0, 1, 2, \ldots\ldots)$ time index

This transformation is described in Appendix A. This is an implicit scheme. It has been chosen implicit in order to insure the numerical stability of the finite difference method without limitation for the time interval Δt.

The coefficients of the system (3-I); (4-I), which are dependent from the unknown fluxes ψ and φ, have been calculated at the time level n - 1. The system is in such a manner linearized. The error introduced by such an approximation is negligible only for small Δt and for coefficients which vary slowly with the time. The choice of Δt is based on a compromise between precision and time of calculation.

At every time step the coefficients are given new values which are determined according to the temperature reaction and the position of the control rods.

The known terms q_{i1} and q_{i2} contain explicitly the values of the fluxes ψ_i^{n-1} and φ_i^{n-1} of the preceding time step. An initial distribution of fluxes ψ_i^o and φ_i^o is given at t = 0.

At every time step the problem is reduced to the solution of the system of 2 x L linear equations in the variables ψ_i and φ_i.

The solution has been obtained with two methods, one iterative and the other direct.

II. Iterative method (Block Gauss-Seidel)

The system (I-3); (I-4) may be written in matrix notation (see page 25 of Appendix A).

$$\begin{cases} A_1 \psi - S \varphi = q_1 \\ -M \psi + A_2 \varphi = q_2 \end{cases} \qquad \text{(II-1)}$$

The iterative method is as follows:

in the source-term $S\varphi$ of system (II-1) we use the vector φ obtained from the calculation of the preceding time step; the system (II-1) is then solved in ψ. The vector ψ is used in the source-term $M\psi$ of system (II-2) and a new vector φ is calculated. This is used in the source term $S\varphi$ of (II-1) and so on.

This method is the same as the block Gauss-Seidel iterative method. In fact let us consider the system $A\chi = q$ formed by the two systems (II-1) and (II-2); where $\chi = \begin{pmatrix} \psi \\ \varphi \end{pmatrix}$ and $q = \begin{pmatrix} q_1 \\ q_2 \end{pmatrix}$, and the matrix A of the coefficient is partitioned as follows:

$$A = L - U = \left[\begin{array}{c|c} A_1 & 0 \\ \hline -M & A_2 \end{array}\right] - \left[\begin{array}{c|c} 0 & S \\ \hline 0 & 0 \end{array}\right] \qquad \text{(II-3)}$$

Applying the block Gauss-Seidel iterative method we have

$$L \cdot \chi^{r+1} = U \cdot \chi^{r} + q$$

which divides into the two subsystems

$$A_1 \psi^{r+1} = S\varphi^r + q_1 \qquad \text{(II-4)}$$

$$-M \psi^{r+1} + A_2 \varphi^{r+1} = q_2 \qquad \text{(II-5)}$$

For a time interval sufficiently small (see Appendix A) the matrix of the coefficients A fulfills the following conditions:

$$a_{ii} > 0 \qquad \text{(II-6)}$$

$$a_{ij} \leq 0 \quad \text{for } i \neq j \qquad \text{(II-7)}$$

$$a_{ii} > \sum_{\substack{j=1 \\ j \neq i}}^{N} |a_{ij}| \qquad \text{(II-8)}$$

which are sufficient to insure the convergence of the iterative method (see Appendix B).

The solution of the systems

$$A_1 \psi^{r+1} = S\varphi^r + q_1 \qquad \text{(II-9)}$$

$$A_2 \varphi^{r+1} = M\psi^{r+1} + q_2 \qquad \text{(II-10)}$$

must be performed at every iteration; this is obtained by a direct method. The systems (II-9) and (II-10), with tri-diagonal matrices A_1 and A_2, are of the type:

$$-r_i \chi_{i-1} + p_i \chi_i - r_{i+1} \cdot \chi_{i+1} = U_i \quad (i=1,\ldots L) \qquad \text{(II-11)}$$

with $$\chi_o = \chi_{L+1} = 0$$

The known terms U_ι contain the source-terms.

The solution of system (II-11) is obtained by using the recursion formula:

$$\chi_\iota = \alpha_\iota \chi_{j+1} + \beta_\iota \tag{II-12}$$

$$\alpha_\iota = \frac{r_{\iota+1}}{p_\iota - r_\iota \alpha_{\iota-1}} \tag{II-13}$$

$$\beta_\iota = \frac{U_\iota + r_\iota \cdot \beta_{\iota-1}}{p_\iota - r_\iota \cdot \alpha_{\iota-1}} \quad \text{with } \alpha_o = \beta_o = 0 \tag{II-14}$$

This recursive method is suitable for the numerical calculation because α_ι and β_ι are of the same magnitude. Only three multiplications, two divisions and three additions are necessary for the calculation of each spatial point.

In our case the matrix fulfills the conditions:

$$r_\iota > 0 \tag{II-15}$$

$$p_\iota > r_\iota + r_{\iota+1} \tag{II-16}$$

Therefore we have:

$$\alpha_\iota < 1 \tag{II-17}$$

the error ε_j resulting from the calculation of χ_j is transmitted by the recursive formula (II-12) according to:

$$\varepsilon_{j-1} = \alpha_{j-1} \cdot \varepsilon_j \tag{II-18}$$

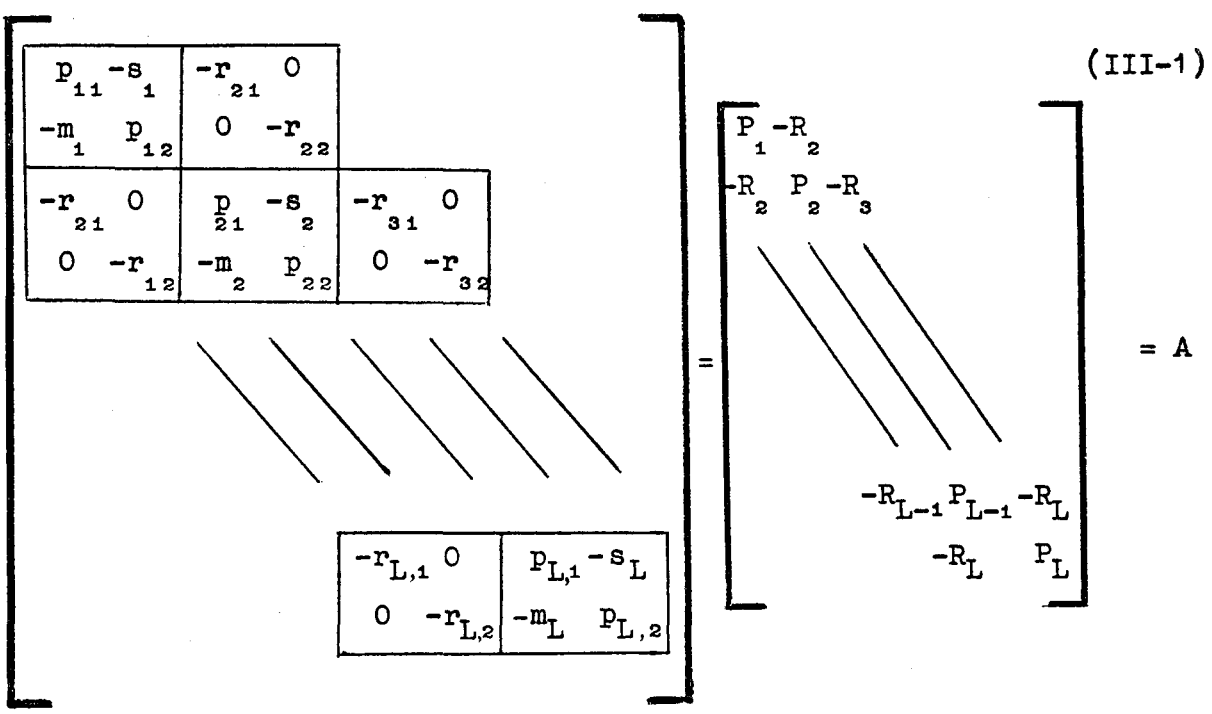
and for (II-17) we have

$$\varepsilon_{j-1} < \varepsilon_j \tag{II-19}$$

The numerical stability is therefore also assured for lattices with a great number of points.

III. The direct method

Rearranging the system (I-3), (I-4), intercalating the equations of (I-3) with the corresponding equations of (I-4), we obtain a system with a pentadiagonal matrix of the coefficients. This matrix can be partitioned into (2 x 2) submatrices according to the following scheme:



(III-1)

The generic equation of the system is:

$$-R_i \cdot \chi_{i-1} + P_i \cdot \chi_i - R_{i+1} \cdot \chi_{i+1} = q_i \qquad (i = 1, \ldots, L) \qquad \text{(III-2)}$$

where

$$\chi_i = \begin{pmatrix} \psi_i \\ \varphi_i \end{pmatrix} \qquad q_i = \begin{pmatrix} q_{i1} \\ q_{i2} \end{pmatrix}$$

and where R_i and P_i are non singular 2 x 2 matrices.

The direct method of solution employed for the equations (II-11), with the recursion formula (II-12), may be generalized for this case of equation (III-3). In fact the matrix A, if considered as consisting of 2 x 2 submatrices, is tridiagonal.

The recursion formulae are now

$$\chi_l = A_l \cdot \chi_{l+1} + b_l \qquad \text{(III-3)}$$

where the matrix A_l is

$$A_l = \left(P_l - R_l \cdot A_{l-1}\right)^{-1} \cdot R_{l+1} \qquad \text{(III-4)}$$

and the vector b_l is

$$b_l = \left(P_l - R_l \cdot A_{l-1}\right)^{-1} \cdot \left(q_l + R_l \cdot b_{l-1}\right) \qquad \text{(III-5)}$$

The boundary conditions are:

$$\chi_o = \chi_{L+1} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

and therefore we have $A_o = 0$ and $b_o = 0$

Starting from A_o and b_o we can calculate forwards all the A_l and b_l, and with these, starting from χ_{L+1}, we can calculate backwards all the χ_l

For this method it is necessary to perform the inversion of the L matrices $(P_l - R_l \cdot A_{l-1})$.

NOTE:

In order to avoid the cumbersome operation of inverting these L (2 x 2) matrices we tried the H-method of Schechter, where it is sufficient to invert only one matrix. The matrices R_i are diagonal and therefore directly invertible. We multiply the system (III-2) by R

$$R = \begin{bmatrix} I & & \\ & R_2^{-1} & \\ & & \ddots \\ & & & R_2^{-1} \end{bmatrix}$$

The matrix of the coefficients then becomes:

$$R \cdot A = \begin{bmatrix} P_1' & R_2' & & & \\ I & P_2' & R_2' & & \\ & I & P_3' & R_3' & \\ & & \ddots & \ddots & \ddots \\ & & & I & P_L' \end{bmatrix}$$

with $P_i' = R_i^{-1} \cdot P_i$; $\quad R_{i+1}' = -R_i^{-1} \cdot R_{i+1}$; $\quad q_1' = R_i^{-1} \cdot q_i$

The recursion formulae of the H-method are:

$$\chi_L = H_L^{-1} \cdot w_L$$

$$\chi_{i-1} = q_i' - P_1'\chi_1 - R_{i+1}' \cdot \chi_{i+1} \qquad (i = L, \ldots, 2)$$

where $$H_i = H_{i-1} \cdot P'_i - H_{i-2} \cdot R'_i$$

$$w_i = H_{i-1} \cdot q_i - w_{i-1}$$

and for the boundary conditions

$$H_o = I \qquad H_1 = P'_1 \qquad w_1 = q_1$$

(See Schechter: "Quasi-Tridiagonal Matrices and Type-insensitive Difference Equations")

With this method, however, we obtain unsatisfactory results because of the propagation of the rounding errors:

$$\varepsilon_{i-1} = -P'_i \cdot \varepsilon_i - R'_{i+1} \cdot \varepsilon_{i+1}$$

IV. Numerical examples

The two methods above described are part of a numerical code to be employed on the IBM 7090, and which is made for the study of the spatio-temporal dynamics of the Reactor TESI. This reactor operates in the following way: from being critical at a very low power it is made prompt critical. The flux rises very rapidly, and, as the reactor is not cooled during the transient, the temperature in the core rises accordingly. The core has a large negative temperature coefficient, therefore when a certain value of the flux is reached the reactor becomes undercritical and the flux decreases very rapidly.

For testing the two methods of calculation we introduce stepwise a reactivity $\rho = 0{,}1$ %. The control rods in this particular case are supposed to be extracted instantaneously and Σp (rod equivalent poison, see page 3) is reduced instantaneously and uniformly all over the core. This causes a transient of the order of 0,5 sec, during which the flux changes from 10^{10} to 10^{18} $\frac{n}{cm^2 sec}$. For a given time interval Δt, chosen for the numerical calculation, the increment of the flux in Δt is very large.

With the iterative method the thermal flux at the time t_n is taken as a first estimate for calculating the fluxes at the time $t_{n+1} = t_n + \Delta t$. Therefore the choice of Δt influences very much the effectiveness of this method: the greater Δt, the greater is the number of inner iterations necessary to reach the wanted precision.

Many tests were made using several Δt in the range:

$$5 \cdot 10^{-5} \text{ sec} \leqslant \Delta t \leqslant 2 \cdot 10^{-3} \text{ sec.}$$

With the direct method and with various Δt contained within these limits the fluxes and temperatures have no appreciable variation. In Fig. 1 are the curves of $\overline{\Phi}(t)$, ($\overline{\Phi}$ is the thermal flux averaged throughout the core). These curves were obtained by both the direct and the iterative method, the iterative method with enough iterations to obtain practically the same results as with the direct method. For Δt less than 10^{-3} sec the curve has no appreciable variation, for $\Delta t > 10^{-3}$ sec the curve tends to be deformed. This is due to the fact that the variation of the temperature-dependent physical parameters during the interval Δt is no longer negligible.

In Fig. 2 are plotted the curves $\Phi(t)$ for $\Delta t = 10^{-3}$ sec, calculated with the direct method and with the iterative method with 2, 3, 4, 5, and 6 iterations. Table 1 contains the numerical values of some points of these curves.

Fig. 3 contains the values of the flux calculated at a transient time value of 0,2 sec. These are plotted against the time interval Δt. The curve of the direct method remains at a constant value for all $\Delta t < 10^{-3}$ sec. The other curves, corresponding to the iterative method, tend to the same value for decreasing Δt. The greater is the number of inner iterations, the greater is the Δt for which the wanted precision is obtained.

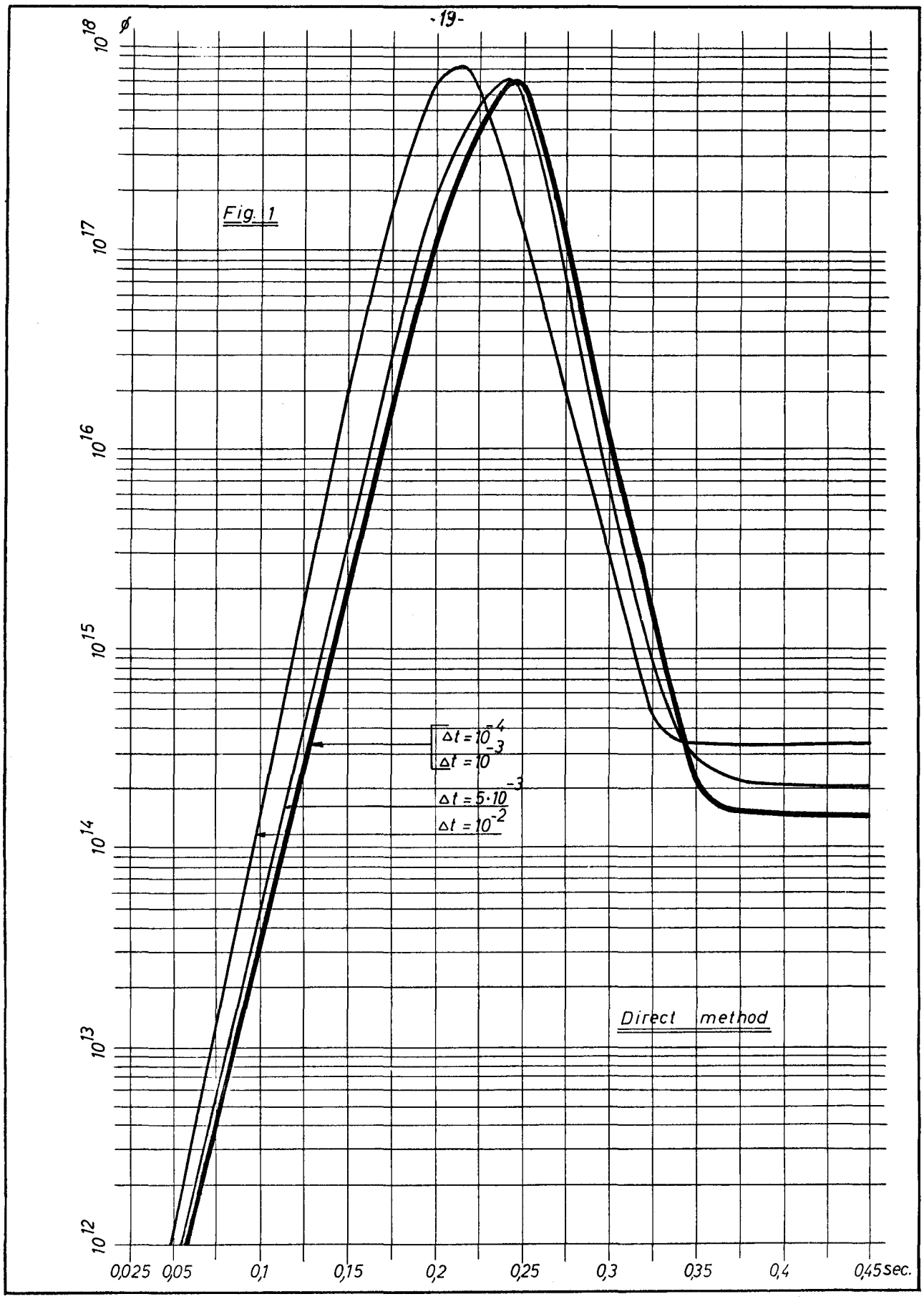
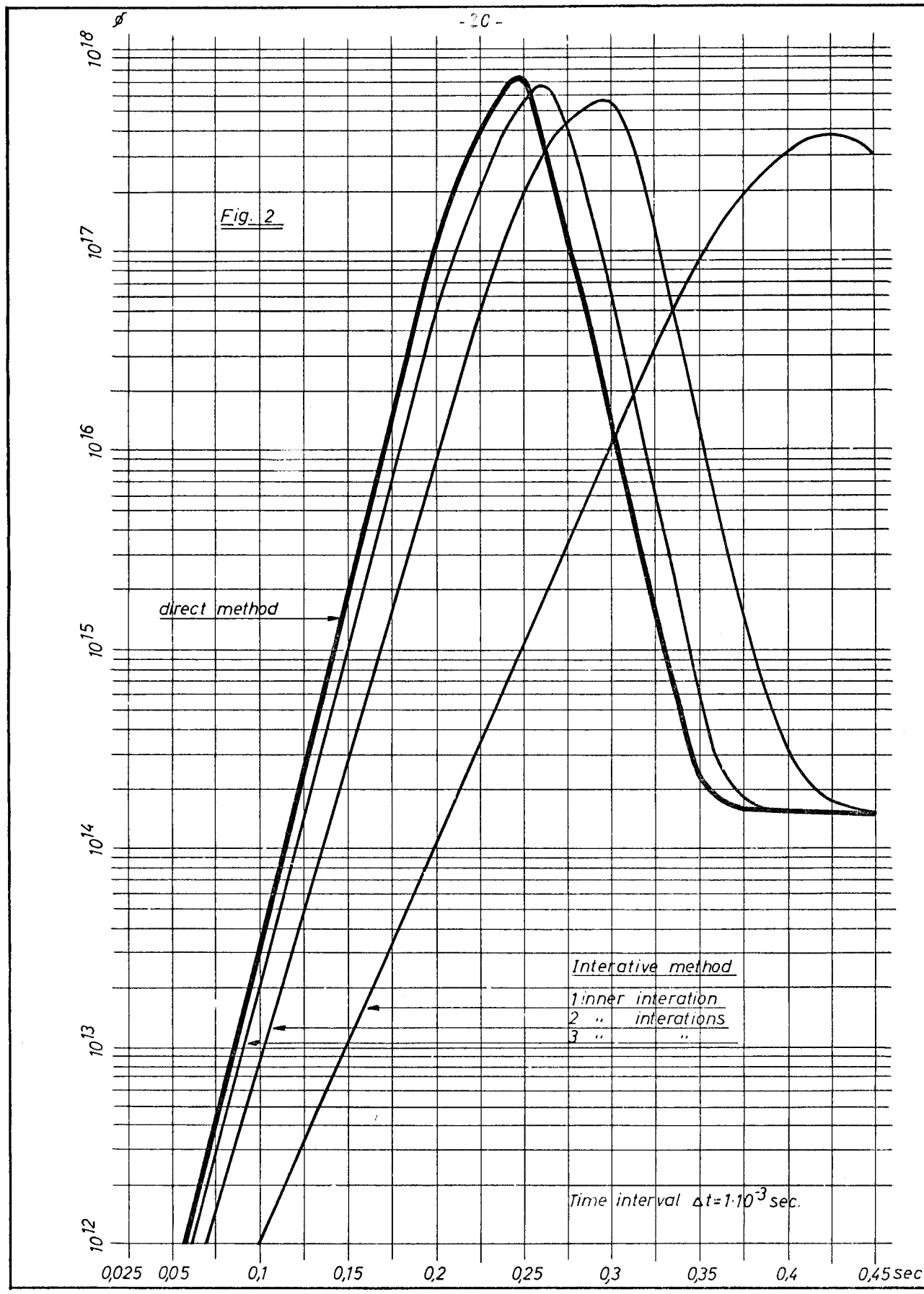


Fig. 1
ϕ
10^{18}
10^{17}
10^{16}
10^{15}
10^{14}
10^{13}
10^{12}
$\Delta t = 10^{-4}$
$\Delta t = 10^{-3}$
$\Delta t = 5 \cdot 10^{-3}$
$\Delta t = 10^{-2}$
Direct method
0,025
0,05
0,1
0,15
0,2
0,25
0,3
0,35
0,4
0,45 sec.


Φ
10^18
10^17
10^16
10^15
10^14
10^13
10^12
Fig. 2
direct method
Interative method
1 inner interation
2 " interations
3 " "
Time interval Δt=1·10^-3 sec.
0,025
0,05
0,1
0,15
0,2
0,25
0,3
0,35
0,4
0,45 sec.

TIME	ITERATIVE METHOD NUMBER OF INNER ITERATIONS					DIRECT METHOD
	2	3	4	5	6	
0.	0.10000E 11	0.10000E 11	0.10000E 11	0.10000E 11	0.10000E 11	0.10000E 11
0.0500	0.32645E 12	0.49922E 12	0.57849E 12	0.60797E 12	0.61816E 12	0.62332E 12
0.1000	0.10089E 14	0.23574E 14	0.31651E 14	0.34959E 14	0.36141E 14	0.36746E 14
0.1500	0.31109E 15	0.11099E 16	0.17254E 16	0.20022E 16	0.21043E 16	0.21572E 16
0.2000	0.94310E 16	0.48360E 17	0.82754E 17	0.98611E 17	0.10448E 18	0.10753E 18
0.2500	0.19746E 18	0.56132E 18	0.64856E 18	0.66439E 18	0.66783E 18	0.66956E 18
0.3000	0.54986E 18	0.58789E 17	0.20634E 17	0.14619E 17	0.13063E 17	0.12359E 17
0.3500	0.14069E 17	0.54414E 15	0.27716E 15	0.23967E 15	0.23035E 15	0.22640E 15
0.4000	0.30090E 15	0.15843E 15	0.15747E 15	0.15760E 15	0.15774E 15	0.15779E 15
0.4500	0.15539E 15	0.15541E 15	0.15626E 15	0.15663E 15	0.15684E 15	0.15690E 15

RESULTS OBTAINED WITH DELTA T = 0.001

TAB. 1

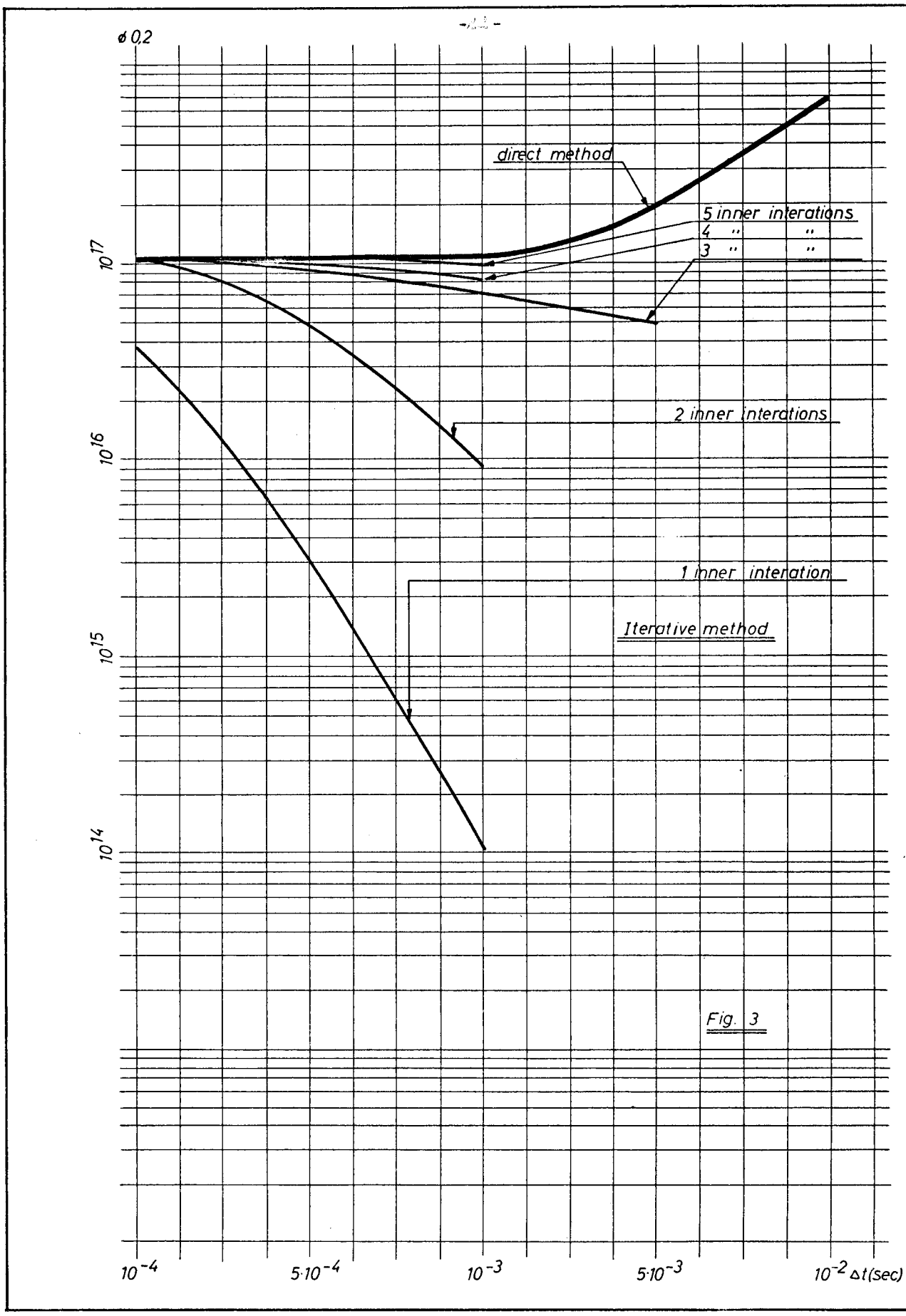

ϕ 0,2
direct method
5 inner interations
4 " "
3 " "
2 inner interations
1 inner interation
Iterative method
10^{17}
10^{16}
10^{15}
10^{14}
10^{-4}
$5 \cdot 10^{-4}$
10^{-3}
$5 \cdot 10^{-3}$
10^{-2} Δt(sec)

Fig. 3

V. Iterative method with variable number of inner iterations

The number of inner iterations necessary to obtain a given precision is proportional to the difference

$$\Delta\bar{\Phi} = \bar{\Phi}\,(t_n + \Delta t) - \bar{\Phi}\,(t_n)$$

But $\Delta\bar{\Phi}$ varies with t_n during the transient. Therefore the program was made to iterate until

$$\frac{\bar{\Phi}^n_i - \bar{\Phi}^n_{i-1}}{\bar{\Phi}^n_i} < \varepsilon$$

where i is the index of the inner iteration and ε is the greatest admissible relative error. The maximum number of allowable iterations is fixed, and when this maximum number is reached the program stops iterating even if the wanted precision is not yet attained. By this method it is possible to avoid a number of useless iterations in some parts of the transient, and, by increasing the max. number of allowable iterations, to reach any wanted precision.

TABLE No. 2

Δt	max. number of iterations	ε	η	time direct	time iterative
$2\cdot10^{-3}$	6	10^{-4}	1,066	23"	38"
$2\cdot10^{-3}$	8	10^{-4}	0,213	23"	44"
10^{-3}	6	10^{-4}	0,0283	41"	1' 03"
$5\cdot10^{-4}$	4	10^{-4}	0,024	1' 15"	1' 32"
10^{-4}	3	10^{-4}	0,00306	5' 48"	5' 44"
10^{-4}	2	10^{-4}	0,05134	5' 48"	4' 46"

TABLE No. 2 contains for various Δt:

max. : The maximum number of allowable iterations.

ε : The relative error at which, when reached, the iterations stop.

η : $\eta = \max_{t>0} \left| \frac{\bar{\Phi}^{it.}(t) - \bar{\Phi}^{dir.}(t)}{\bar{\Phi}^{dir.}(t)} \right|$

where $\bar{\Phi}^{it.}$ and $\bar{\Phi}^{dir.}$ are the fluxes calculated respectively with the iterative and the direct method.

time direct : The calculating time of the direct method.

time iterative: The calculating time of the iterative method.

Appendix A

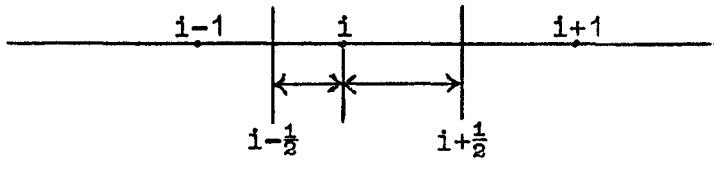
The diffusion equations of the R_k region are:

$$D_f^k \frac{\partial^2}{\partial z^2} \psi - A^k \psi + B^k \varphi + C^k = \frac{1}{w^k} \frac{\partial \psi}{\partial t} \qquad (a\text{-}1)$$

$$D_t^k \frac{\partial^2}{\partial z^2} \varphi - E^k \varphi + F^k \psi = \frac{1}{v^k} \frac{\partial \varphi}{\partial t} \qquad (a\text{-}2)$$

The space is divided into mesh-points $\{z_i\}$ $(i=0, 1, 2, \ldots L, L+1)$. On each interface between two regions is a point of the lattice, and each region contains at least one point.

The mesh increment is $\Delta_i = z_{i+1} - z_i$. For all the points $i=1, 2, \ldots L$ the equations (a-1) and (a-2) must be integrated in the intervals $z_{i-\frac{1}{2}} \leqslant z \leqslant z_i$ and $z_i \leqslant z \leqslant z_{i+\frac{1}{2}}$



For the sake of brevity only the integration of equation (a-1) is reported here:

$$\int_{z_{i-\frac{1}{2}}}^{z_i} \frac{1}{w} \frac{\partial \psi}{\partial t} \cdot dz = \left[D_f \frac{\partial \psi}{\partial z} \right]_{z_i -} - \left[D_f \frac{\partial \psi}{\partial z} \right]_{z_{i-\frac{1}{2}}} - \int_{z_{i-\frac{1}{2}}}^{z_i} (A \cdot \psi - B \cdot \varphi - C)\, dz \qquad (a\text{-}3)$$

$$\int_{z_l}^{z_{l+\frac{1}{2}}} \frac{1}{w}\frac{\partial\psi}{\partial t}\cdot dz = \left[D_f \frac{\partial\psi}{\partial z}\right]_{z_{l+\frac{1}{2}}} - \left[D_f \frac{\partial\psi}{\partial z}\right]_{z_{l+}} - \int_{z_l}^{z_{l+\frac{1}{2}}} (A\cdot\psi - B\cdot\varphi - C)\, dz \qquad (a\text{-}4)$$

where

$$\left[f(z)\right]_{z_{l-}} \quad \text{and} \quad \left[f(z)\right]_{z_{l+}}$$

are respectively the left and right limit of $f(z)$ in $z = z_l$.

Adding (a-3) and (a-4) and remembering that fluxes and currents are continuous we have:

$$\int_{z_{l-\frac{1}{2}}}^{z_{l+\frac{1}{2}}} \frac{1}{w}\frac{\partial\psi}{\partial t} = \left[D_f \frac{\partial\psi}{\partial z}\right]_{z_{l+\frac{1}{2}}} - \left[D_f \frac{\partial\psi}{\partial z}\right]_{z_{l-\frac{1}{2}}} - \int_{z_{l-\frac{1}{2}}}^{z_{l+\frac{1}{2}}} (A\cdot\psi - B\cdot\varphi - C)\, dz \qquad (a\text{-}5)$$

The derivatives $\frac{\partial\psi}{\partial z}$ are calculated with central differences; the integrals are approximated according to the formula:

$$\int_{z_{l-\frac{1}{2}}}^{z_{l+\frac{1}{2}}} f(z)\, dz = f_l^- \cdot \frac{\Delta_{l-1}}{2} + f_l^+ \cdot \frac{\Delta_l}{2} \qquad (a\text{-}6)$$

The derivatives with respect to the time are approximated according to:

$$\left[\frac{\partial\psi}{\partial t}\right]_{z_l} = \frac{\psi(z_l, t) - \psi(z_l, t-\Delta t)}{\Delta t} = \frac{\psi_l^n - \psi_l^{n-1}}{\Delta t} \qquad (a\text{-}7)$$

Equation (a-5) then becomes:

$$0 = \left[\frac{1}{w}\frac{\psi^n - \psi^{n-1}}{\Delta t}\right]_{z_l-} \cdot \frac{\Delta_{l-1}}{2} + \left[\frac{1}{w}\frac{\psi^n - \psi^{n-1}}{\Delta t}\right]_{z_l+} \cdot \frac{\Delta_l}{2} - D_{l+\frac{1}{2}} \frac{\psi^n_{l+1} - \psi^n_l}{\Delta_l} +$$

$$D_{l-\frac{1}{2}} \frac{\psi^n_l - \psi^n_{l-1}}{\Delta_{l-1}} + \left[A \cdot \psi^n - B \cdot \varphi^n - C\right]_{z_l-} \cdot \frac{\Delta_{l-1}}{2} + \left[A \cdot \psi^n - B \cdot \varphi^n - C\right]_{z_l+} \cdot \frac{\Delta_l}{2}$$

(a-8)

If z_l is a point internal to R_k then $D_{f_{l-\frac{1}{2}}} = D_{f_{l+\frac{1}{2}}} = D^k_f$.
The functions A, B, C are continuous in z_l and equation (a-8) therefore becomes:

$$-\frac{D^k_f}{\Delta_{l-1}} \psi^n_{l-1} + \left[D^k_f \left(\frac{1}{\Delta_{l-1}} + \frac{1}{\Delta_l}\right) + \left(\frac{1}{w^k_l \cdot \Delta t} + A^k_l\right) \cdot \left(\frac{\Delta_{l-1} + \Delta_l}{2}\right)\right] \psi^n_l -$$

(a-9)

$$-\frac{D^k_f}{\Delta_l} \psi^n_{l+1} - \left[B^k_l \frac{\Delta_{l-1} + \Delta_l}{2}\right] \varphi^n_l = \left[C^k_l + \frac{\psi^{n-1}_l}{w^k_l \cdot \Delta t}\right] \left(\frac{\Delta_{l-1} + \Delta_l}{2}\right)$$

If z_l is a point on the interface between R_{k-1} and R_k it is

$$D_{f_{l-\frac{1}{2}}} = D^{k-1}_f \qquad D_{f_{l+\frac{1}{2}}} = D^k_f$$

$$(A)_{z_l-} = A^{k-1}_l \qquad (A)_{z_l+} = A^k_l \quad ,$$

same for B, C, w.

Equation (a-8) therefore becomes:

$$- \frac{D_f^{k-1}}{\Delta_{i-1}} \psi_{i-1}^n + \left[\frac{D_f^{k-1}}{\Delta_{i-1}} + \frac{D_f^k}{\Delta_i} + \left(\frac{1}{w_i^{k-1} \Delta t} + A_i^{k-1} \right) \frac{\Delta_{i-1}}{2} + \right.$$

$$\left. + \left(\frac{1}{w_i^k - \Delta t} + A_i^k \right) \frac{\Delta_i}{2} \right] \psi_i^n - \frac{D_f^k}{\Delta_i} \psi_{i+1}^n - \left(\frac{B_i^{k-1} \cdot \Delta_{i-1}}{2} + \frac{B_i^k \cdot \Delta_i}{2} \right) \varphi_i^n =$$

$$= \left[C_i^{k-1} + \frac{\psi_i^{n-1}}{w_i^{k-1} \cdot \Delta t} \right] \frac{\Delta_{i-1}}{2} + \left[C_i^k + \frac{\psi_i^{n-1}}{w_i^k - \Delta t} \right] \frac{\Delta_i}{2} \qquad \text{(a-10)}$$

Integrating equation (a-2) with the same proceedings we obtain the two following expressions:

for z_i internal to R_k:

$$- \frac{D_t^k}{\Delta_{i-1}} \cdot \varphi_{i-1}^n + \left[D_t^k \left(\frac{1}{\Delta_{i-1}} + \frac{1}{\Delta_i} \right) + \left(\frac{1}{v_i^k \cdot \Delta t} + E_i^k \right) \cdot \left(\frac{\Delta_{i-1} + \Delta_i}{2} \right) \right] \cdot \varphi_i^n -$$

$$- \frac{D_t^k}{\Delta_i} \varphi_{i+1}^n - \left[F_i^k \cdot \frac{\Delta_{i-1} + \Delta_i}{2} \right] \psi_i^n = \frac{\varphi_i^n}{v_i^k \cdot \Delta t} \cdot \frac{\Delta_{i-1} + \Delta_i}{2} \qquad \text{(a-11)}$$

for z_i on the interface between R_{k-1} and R_k:

$$- \frac{D_t^{k-1}}{\Delta_{i-1}} \cdot \varphi_{i-1}^n + \left[\frac{D_t^{k-1}}{\Delta_{i-1}} + \frac{D_t^k}{\Delta_i} + \left(\frac{1}{v_i^{k-1} \cdot \Delta t} + E_i^{k-1} \right) \cdot \frac{\Delta_{i-1}}{2} + \right.$$

$$\left. + \left(\frac{1}{v_i^k \cdot \Delta t} + E_i^k \right) \cdot \frac{\Delta_i}{2} \right] \cdot \varphi_i^n - \frac{D_t^k}{\Delta_i} \cdot \varphi_{i+1}^n - \left(F_i^{k-1} \frac{\Delta_{i-1}}{2} + F_i^k \cdot \frac{\Delta_i}{2} \right) \cdot \psi_i^n =$$

$$= \frac{\varphi_i^{n-1}}{v_i^{k-1} \cdot \Delta t} \cdot \frac{\Delta_{i-1}}{2} + \frac{\varphi_i^{n-1}}{v_i^k \cdot \Delta t} \cdot \frac{\Delta_i}{2} \qquad \text{(a-12)}$$

The finite-difference equations obtained by this method are of the type:

$$- r_{i1} \psi_{i-1} + p_{i1} \psi_i - t_{i1} \psi_{i+1} - s_i \varphi_i = q_{i1} \qquad \text{(a-13)}$$

$$- m_i \psi_i - r_{i2} \varphi_{i-1} + P_{i2} \varphi_i - t_{i2} \varphi_{i+1} = q_{i2} \qquad \text{(a-14)}$$

$$(i = 1, \ldots, L)$$

where

$$r_{11} = t_{L,1} = r_{12} = t_{L,2} = 0$$

and $t_{i,1} = r_{i+1,1}$ and $t_{i,2} = r_{i+1,2}$

The matrix of the coefficients of the system (a-13) and (a-14) is then:

$$A = \left[\begin{array}{c|c} A_1 & -S \\ \hline -M & A_2 \end{array}\right] = \left[\begin{array}{cccccc|cccccc} p_{11} & -r_{21} & & & & & -s_1 & & & & & \\ -r_{21} & p_{21} & -r_{31} & & & & & -s_2 & & & & \\ & \ddots & \ddots & \ddots & & & & & \ddots & & & \\ & & -r_{L-1,1} & p_{L-1,1} & -r_{L,1} & & & & & -s_{L-1} & & \\ & & & -r_{L,1} & p_{L,1} & & & & & & -s_L & \\ \hline -m_1 & & & & & & p_{12} & -r_{22} & & & & \\ & -m_2 & & & & & -r_{22} & p_{22} & -r_{32} & & & \\ & & \ddots & & & & & \ddots & \ddots & \ddots & & \\ & & & -m_{L-1} & & & & & -r_{L-1,2} & p_{L-1,2} & -r_{L,2} & \\ & & & & -m_L & & & & & -r_{L,2} & p_{L,2} & \end{array}\right]$$

where the entries on the main diagonal are all positive; and all the other entries are $\leqslant 0$.

The tridiagonal matrices A_1 and A_2 are definite positive as they are symmetrical and as their diagonals are dominant and with positive entries.

The diagonal matrices S and M are non-negative.

In order that the entries of the main diagonal of the total matrix A are strictly dominant it is sufficient that

$$\frac{1}{w_i^k \cdot \Delta t} + A_i^k > B_i^k \qquad \text{(a-15)}$$

$$\frac{1}{v_i^k \cdot \Delta t} + E_i^k > F_i^k \qquad \text{(a-16)}$$

This condition is normally satisfied.

Appendix B

Here below are some definitions and theorems necessary to demonstrate that the iterative method (Block-Gauss-Seidel) converges.

Def. 1: It is called "Spectral Radius" $\rho(A)$, the greatest modulus of the proper values of the matrix A:

$$\rho(A) = \max_{i = 1,\ N} |\lambda_i|$$

Def. 2: A matrix A is:

2.a Convergent if the sequence of matrices A, A^2, A^3,... converges to the null matrix 0.

2.b Non negative - $A \geqslant 0$ if all the entries are real and $a_{ij} \geqslant 0$.

2.c Strictly diagonally dominant if for all i = 1,....,N it is

$$|a_{ii}| > \sum_{\substack{i=1 \\ i \neq j}}^{N} |a_{ij}| \ , \qquad (2.c\text{-}1)$$

from (2.c-1) follows evidently

$$\sum_{\substack{i=1 \\ i \neq j}}^{N} \left| \frac{a_{ij}}{a_{ii}} \right| < 1 \ .$$

Def. 3: The splitting of a matrix A

$$A = E - F$$

is a regular splitting if E is a non-singular matrix with $E^{-1} \geqslant 0$ and if $F \geqslant 0$.

Theorem 1 - The necessary and sufficient condition for A to be convergent is:

$$\rho(A) < 1$$

Theorem 2 - The spectral radius $\rho(A)$ of an arbitrary matrix A fulfills the relation

$$\rho(A) \leqslant \max_{i=1,N} \sum_{j=1}^{N} |a_{ij}|$$

Corollary - Let A be a strictly diagonally dominant matrix; let D be a diagonal matrix $D = (\frac{1}{a_{ii}})$, then the matrix $B = I - DA$ is convergent.

In fact the following relation is fulfilled:

$$\rho(B) \leqslant \max_{i=1,N} \sum_{\substack{j=1 \\ j \neq i}}^{N} \left| \frac{a_{ij}}{a_{ii}} \right| < 1$$

Theorem 3 - Let A be a real matrix with $a_{ij} \leqslant 0$ (for $i \neq j$) and $a_{ii} > 0$, and let D be a diagonal matrix $D = (\frac{1}{a_{ii}})$; if the non negative matrix $B = I - DA$ is convergent then A is non-singular and $A^{-1} \geqslant 0$.

Theorem 4 - If $A = E - F$ is a regular splitting of the matrix A and $A^{-1} \geqslant 0$ then

$$\rho\,(E^{-1} \cdot F) = \frac{\rho\,(A^{-1}F)}{1 + \rho\,(A^{-1}F)} < 1$$

Therefore the matrix $E^{-1} \cdot F$ is convergent and the iterative method

$$E\chi^{r+1} = F\chi^{r} + q$$

converges for any initial vector χ^{o}.

This last theorem is interesting for our case. In fact the matrix A of the system in study fulfills the following conditions:

$$a_{ij} \leqslant 0 \quad i \neq j$$

$$a_{ii} > 0$$

$$a_{ii} > \sum_{\substack{j=1 \\ j \neq i}}^{N} |a_{ij}|$$

(see II. page 6)

therefore, for theorem 3, $A^{-1} \geqslant 0$.

The splitting $A = L - U$ is regular, because the following conditions are fulfilled:

$$u_{ij} \geqslant 0 \quad \text{i.e.} \quad U \geqslant 0$$

$$l_{ii} > 0 \qquad l_{ij} \leqslant 0 \quad j \neq i$$

(see II. page 5)

$$l_{ii} > \sum_{\substack{j=1 \\ j \neq i}}^{N} |l_{ij}|$$

and, again for theorem 3, they give $L^{-1} \geqslant 0$.

Therefore, for theorem 4 the iterative method of II. is convergent.

(The theorems 1, 2, 3, 4 are respectively the theorems 1.4, 1.5, 3.10, 3.13 in "Matrix Iterative Analysis" by R. VARGA - Prentice-Hall, Inc.).

References

AIREK: "Generalized Reactor Kinetics Code"; Atomics International, No. 4980.

COHEN, E.R.: "Some Topics in Reactor Kinetics"; Geneva Conference 1958, Volume 11, P/629 USA.

FOX, L: "Numerical Solution of Ordinary and Partial Differential Equations"; Pergamon Press - 1962.

KAPLAN, S.: "Some New Methods of Flux Synthesis"; N.S.&E. 13 - 1962.

P.D.Q.: "An IBM-704 Code to solve the Two-dimensional Few-Group Neutron Diffusion Equations"; WAPD-TM-70.

RICHTMYER, R.D.: "Difference Methods for Initial-Value Problems"; Interscience Publishers, Inc., New York.

SCHECHTER, S.: "Quasi-Tridiagonal Matrices and Type-insensitive Difference Equations; AEC Computing and Applied Mathematics Center - TID-4500, NYO-2542.

STAB: "A Kinetic, Three-Dimensional, One-Group Digital Computer Program"; AEEW-R.77.

VARGA , R.S.: "Matrix Iterative Analysis"; Prentice-Hall, Inc.

WACHSPRESS, E.L.: "Digital Computation of Space-Time Variation of Neutron Fluxes"; KAPL - 2090.

WANDA: "A One-dimensional Few-Group Diffusion Equation Code for the IBM-704".