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NUMERICAL SOLUTION OF THE ONE-GROUP, SPACE-INDEPENDENT REACTOR KINETICS EQUATIONS FOR NEUTRON DENSITY GIVEN THE EXCESS REACTIVITY

by

J. J. Kaganove

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GIVEN THE EXCESS REACTIVITY

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ABSTRACT

The advantages and shortcomings of the codes currently in use at Argonne (RE-13 and RE-129) are discussed. A new method of solution, which has increased accuracy, stability for exceptionally large integration intervals, and a procedure for automatically changing the integration interval as the nature of the problem changes, is developed.

I. Solution for Neutron Density, Given Excess Reactivity.

There has been a continuing interest in developing a versatile digital computer code for solving the one-group, space-independent reactor kinetics equation:

$$\dot{n} = \frac{(1 - \beta)k_{ex} - \beta}{\ell} n + \sum_i \lambda_i c_i + S, \quad (1)$$

or alternately,

$$\left. \begin{aligned} \dot{n} &= \frac{k_{ex}}{\ell} n - \sum_i \dot{c}_i + S \\ \dot{c}_i &= -\lambda_i c_i + \frac{\beta_i}{\ell} (1 + k_{ex}) n \\ k_{ex} &= f(n, t) \end{aligned} \right\}, \quad (1a)$$

where:

$\dot{n}$ = neutron density

$\dot{c}_i$ = concentration of i'th delayed neutron precursor

β = total fraction of delayed neutrons

β_i = total fraction of delayed neutrons of the i'th, group $\left(\sum_i \beta_i = \beta \right)$

λ_i = decay constant for the i'th group

S = constant source term

k_{ex} = excess reactivity = $k_{effective} - 1$

t = time

ℓ = effective prompt neutron lifetime

Most methods employed in computation in the step-by-step integration of differential equations have an essential feature in common, i.e., that at each step use is made of the function values already obtained in preceding steps. Thus, having the value of n_j and wishing to obtain n_{j+1} , these methods require a knowledge of n_{j-1} , n_{j-2} , the number of values depending on the method and the accuracy required. These methods have the advantage of using the available values of n_{j-1} , n_{j-2} to carry information about the behaviour of n in the region of n_j . There are, however, several disadvantages. First, the processes are not self-starting. Two or more consecutive values of n are required; these must be obtained by an auxiliary process. Secondly, it is not always a simple matter to change interval sizes in the middle of a problem. These considerations become even more of a drawback when the problem of coding separate instructions for starting, running solution, and interval changing is considered.

From the preceding discussion it seemed that one of the Runge-Kutta methods would suit our purpose. They possess the advantage that they are self-starting, do not require previous values or higher derivatives of the dependent variables, and a change in spacing is easily effected at any intermediate stage of the calculation. On the other hand, the estimation of error is less simply accomplished than with the previously mentioned methods.

The solution of the kinetics equations was coded at Argonne (designated RE-13) using a fourth-order Runge-Kutta method. It became apparent that the nature of the equation imposed severe limitations on the interval size, especially in the case of fast reactors. R. O. Brittan notes that

"Unfortunately, the presence of the prompt neutron lifetime in the problem, which becomes very small for fast reactors, and the necessity of performing subtractions yielding small differences between large numbers limits the interval size to about $10^3 \ell$. Thus, for classes of problems in which the variables change slowly with time, the number of points which must be computed can become enormous."¹

II. RE-29 Method

Because of the severe limitations on interval size, a method designated as RE-29 (or as RE-129 for use with IBM-704) was developed by R. O. Brittan. The methods can be described as follows:

¹R. O. Brittan, Some Problems in the Safety of Fast Reactors, ANL-5577, p. 6

Integrating eq. (1a) term by term we have,

$$\left. \begin{aligned} n &= n_j + \frac{1}{\ell} \int_0^t k_{ex} n \, dt - \sum_i (c_i - c_{ij}) + St \\ c_i &= c_{ij} - \lambda_i \int_0^t c_i \, dt + \frac{\beta_i}{\ell} \int_0^t (1 + k_{ex}) n \, dt \end{aligned} \right\}, \quad (2)$$

where t is measured from the beginning of the j 'th interval. The excess reactivity is assumed to vary linearly with time in the interval, i.e.,

$$k_{ex} = k_{ex,j} + \frac{\Delta k}{\Delta t} t, \quad (3)$$

where

$$\Delta k = k_{ex,j+1} - k_{ex,j} = k_{ex}(\Delta t) - k_{ex}(0). \quad (4)$$

If we now replace any dependent variable that appears under an integral with a polynomial approximation, integrate, and then determine the unknown coefficients in a suitable fashion, we then have an approximate solution over the interval.

In particular, if the choice of the polynomial approximations is restricted to being linear and the coefficients are determined such that eq. (2) is satisfied for ($t = 0$, $t = \Delta t$), we have for each interval:

$$\Delta n = n_{j+1} - n_j = \frac{n_j \frac{\Delta t}{\ell} \left[k_{ex,j} + \frac{\Delta k}{2} (1 - \Sigma^*) \right] - \sum_i \left[\frac{\left(\frac{dc_i}{dt} \right)_j \Delta t}{1 + \lambda_i \frac{\Delta t}{2}} \right] + S \Delta t}{1 - \frac{\Delta t}{2\ell} \left[\left(k_{ex,j} + \frac{2\Delta k}{3} \right) (1 - \Sigma^*) - \Sigma^* \right]}, \quad (5)$$

where

$$\Sigma^* = \sum_i \frac{\beta_i}{1 + \frac{1}{2} \lambda_i \Delta t}$$

and

$$\Delta c_i = c_{i,j+1} - c_{ij} = \frac{\frac{\beta_i}{\ell} \left[n_j \Delta k + \Delta n \left(1 + k_{ex,j} + \frac{2\Delta k}{3} \right) \right] \frac{\Delta t}{2} + \left(\frac{dc_i}{dt} \right)_j \Delta t}{\left(1 + \frac{1}{2} \lambda_i \Delta t \right)}. \quad (6)$$

The solution is then obtained by the successive evaluations of eq. (5) and (6) for each interval. Excess reactivity is determined for each interval by a subroutine which includes an iteration method for use when the reactivity is a function of the neutron density as well as time.

In addition to providing a method of circumventing the problems of small differences between large numbers in the Runge-Kutta method, RE-29 has other advantages when short prompt lifetimes are considered. An examination from a macroscopic viewpoint of the solution of the equations for ramp (linear) or approximate ramp insertions of reactivity shows an apparent discrepancy in behavior in the neighborhood of the origin. Graphs of the solutions seem to indicate a discontinuity of $\dot{n}$ near the origin although the equations show that, since k_{ex} is continuous, $\dot{n}$ must also be continuous. A closer examination of the solution shows extremely rapid changes of $\dot{n}$ in the interval between the origin and about 100-200 prompt lifetimes. If a solution is attempted by means of the Runge-Kutta methods, time intervals no greater than 10ℓ or $10^2\ell$ must be employed because of the strong dependence of the method on the value of the first derivative at the beginning of the interval. Method RE-29, on the other hand, has a weaker dependence on the value of $\dot{n}$ at the beginning of the interval and thus much more readily handles the case where k_{ex} is discontinuous.

There are, however, several drawbacks to RE-29. This procedure was originally developed for use on the AVIDAC, which necessitated certain simplifications because of the limited storage capacity of the machine. The approximation of k_{ex} by linear segments is obviously too crude for many applications, requiring very short time intervals. When the excess reactivity is in the neighborhood of prompt critical, RE-29 has no advantage over the Runge-Kutta methods. The solutions in this region reveal the neutron density to be varying rapidly, so that the integration interval must be cut to the size where the Runge-Kutta method may be used with a somewhat better accuracy.

If eq. (2) are combined together, the linear approximations are substituted under the integral sign, and the integration carried out, there is obtained

$$\begin{aligned}
 n = n_j + & \left[\frac{(1-\beta)k_{ex,j} - \beta}{\ell} n_j + \sum_i \lambda_i c_{ij} + S \right] \frac{t}{1!} \\
 & + \left[\frac{(1-\beta)k_{ex,j} - \beta}{\ell} \frac{\Delta n}{\Delta t} \frac{(1-\beta)}{\ell} n_j \frac{\Delta k}{\Delta t} + \sum_i \lambda_i \frac{\Delta c_i}{\Delta t} \right] \frac{t^2}{2!} \\
 & + \left[2 \frac{1-\beta}{\ell} \frac{\Delta k}{\Delta t} \frac{\Delta n}{\Delta t} \right] \frac{t^3}{3!} .
 \end{aligned} \tag{7}$$

If eq. (7) is compared with the Taylor expansion of n , it will be seen that the coefficient of t is the same in both cases, i.e., $\dot{n}_j$. The coefficient of $t^2/2!$ in eq. (7) is the expression for $\ddot{n}_j$ with $\dot{n}_j$, c_j , and $k_{ex,j}$ replaced by the terms $\Delta n/\Delta t$, $\Delta c_j/\Delta t$, and $\Delta k/\Delta t$, respectively. These are obtained from eqs. (5) and (6) and the assumption of linearity of k_{ex} . The coefficient of $t^3/3!$ similarly corresponds to $\dddot{n}_j$, but with the terms involving $\dot{n}_j$, $k_{ex,j}$, and c_{ij} taken to be zero. One would expect trouble when $\ddot{n}$ becomes large and in practice this has been so. Instabilities occur in the vicinity of sharp peaks where the second derivative is large unless the interval size is chosen suitably small.

Attempts to use RE-29 for operational problems in which n is varying very slowly have indicated an upper limit of interval size which is independent of the prompt lifetime. When using the Hughes' data for the precursor equations, this upper limit seems to be in the neighborhood of $\Delta t = 0.1$ sec. As a partial explanation of this behavior, consider the reduced precursor equations:

$$\dot{c}_i + \lambda_i c_i = 0 \quad (8)$$

The solutions to eq. (8) are

$$c_i = c_{ij} e^{-\lambda_i t} \quad (9)$$

or, alternately,

$$\Delta c_i = c_i(\Delta t) - c_{ij} = c_{ij} (e^{-\lambda_i \Delta t} - 1) \quad (10)$$

If the method of RE-29 is applied to eq. (8), there is obtained

$$\bar{c}_i = c_{ij} \left(\frac{-\lambda_i \Delta t}{1 - \frac{1}{2} \lambda_i \Delta t} \right) \quad (11)$$

It is interesting to note that the error in eq. (11) is bounded as $\lambda_i \Delta t \rightarrow \infty$. The error for $\lambda_i \Delta t = 0.1$ is 0.08%, but increases rapidly to 5.5% for $\lambda_i \Delta t = 1.0$. Using the largest value of λ of the Hughes' data ($\lambda_m = 14.3$) and the previously mentioned Δt of 0.1 sec, the error is 10.9%.

Because of the limitations of the preceding methods, a new method of solution would seem desirable. The following method has the desirable features of RE-29 without the shortcomings previously described.

III. Proposed Method

Consider, first, the precursor equations of eq. (1a). Advantage may be taken of the relative simplicity in the dependent variable, i.e., linear in $\dot{c}_i$ and c_i with constant coefficients. The solutions for c_i in terms of a functional of the neutron density is

$$c_i - c_{ij} = -c_{ij} (1 - e^{-\lambda_i t}) + \frac{\beta_i}{\ell} \int_0^t e^{-\lambda_i(t-\tau)} (1 + k_{ex}) n d\tau \quad (12)$$

If the neutron density equation of the set (1a) is integrated term-by-term,

$$n - n_j = \int_0^t \frac{k_{ex} n}{\ell} dt - \sum_i (c_i - c_{ij}) + St \quad (13)$$

Upon substitution of eq. (12) into eq. (13), there is obtained

$$\begin{aligned} n - n_j = & \int_0^t \frac{k_{ex} n}{\ell} dt - \sum_i \frac{\beta_i}{\ell} \int_0^t e^{-\lambda_i(t-\tau)} (1 + k_{ex}) n d\tau \\ & + \sum_i c_{ij} (1 - e^{-\lambda_i t}) + St \quad (14) \end{aligned}$$

(If k_{ex} is considered to be a function of time only, then eq. (14) is a Volterra integral equation of the second kind.)

For any interval under consideration, let

$$k_{ex} = k_{ex,j} + \frac{k_1}{\Delta t} t + \frac{k_2}{(\Delta t)^2} t^2 \quad (15)$$

and

$$n = n_j + \frac{n_1}{\Delta t} t + \frac{n_2}{(\Delta t)^2} t^2 \quad (16)$$

If eqs. (15) and (16) are substituted into eq. (14) and then the conditions are imposed that the integral equation be satisfied at the midpoint and end of the interval, there is obtained, after rearranging terms, two equations for the unknowns n_1 and n_2 :

$$\begin{aligned} & \left\{ 1 - \frac{\Delta t}{\ell} \left[\frac{k_{ex,j}}{2} - (1 + k_{ex,j}) \sum_i \beta_i I_{i1}(\Delta t) + k_1 \left(\frac{1}{3} - \sum_i \beta_i I_{i2}(\Delta t) \right) + k_2 \left(\frac{1}{4} - \sum_i \beta_i I_{i3}(\Delta t) \right) \right] \right\} n_1 \\ & + \left\{ 1 - \frac{\Delta t}{\ell} \left[\frac{k_{ex,j}}{3} - (1 + k_{ex,j}) \sum_i \beta_i I_{i2}(\Delta t) + k_1 \left(\frac{1}{4} - \sum_i \beta_i I_{i3}(\Delta t) \right) + k_2 \left(\frac{1}{5} - \sum_i \beta_i I_{i4}(\Delta t) \right) \right] \right\} n_2 \\ & = \frac{\Delta t}{\ell} \left\{ n_j \left[k_{ex,j} + k_1 \left(\frac{1}{2} - \sum_i \beta_i I_{i1}(\Delta t) \right) + k_2 \left(\frac{1}{3} - \sum_i \beta_i I_{i2}(\Delta t) \right) \right] - \sum_i \ell \dot{c}_{ij} I_{i0}(\Delta t) \right\} + S \Delta t \quad (17) \end{aligned}$$

$$\begin{aligned}
& \left\{ \frac{1}{2} - \frac{\Delta t}{\ell} \left[\frac{k_{ex,j}}{8} - \left(\frac{1 + k_{ex,j}}{2} \right) \sum_i \beta_i I_{i1} \left(\frac{\Delta t}{2} \right) + k_1 \left(\frac{1}{24} - \frac{1}{4} \sum_i \beta_i I_{i2} \left(\frac{\Delta t}{2} \right) \right) + k_2 \left(\frac{1}{64} - \frac{1}{8} \sum_i \beta_i I_{i3} \left(\frac{\Delta t}{2} \right) \right) \right] \right\} n_1 \\
& + \left\{ \frac{1}{4} - \frac{\Delta t}{\ell} \left[\frac{k_{ex,j}}{24} - \left(\frac{1 + k_{ex,j}}{4} \right) \sum_i \beta_i I_{i2} \left(\frac{\Delta t}{2} \right) + k_1 \left(\frac{1}{64} - \frac{1}{8} \sum_i \beta_i I_{i3} \left(\frac{\Delta t}{2} \right) \right) + k_2 \left(\frac{1}{160} - \frac{1}{16} \sum_i \beta_i I_{i4} \left(\frac{\Delta t}{2} \right) \right) \right] \right\} n_2 \\
& = \frac{\Delta t}{\ell} \left\{ n_j \left[\frac{k_{ex,j}}{2} + k_1 \left(\frac{1}{8} - \frac{1}{2} \sum_i \beta_i I_{i1} \left(\frac{\Delta t}{2} \right) \right) + k_2 \left(\frac{1}{24} - \frac{1}{4} \sum_i \beta_i I_{i2} \left(\frac{\Delta t}{2} \right) \right) \right] - \sum_i \ell \dot{c}_{ij} I_{i0} \left(\frac{\Delta t}{2} \right) \right\} + \left(\frac{\Delta t}{2} \right) S \quad (18)
\end{aligned}$$

where

$$\dot{c}_{ij} = -\lambda_i c_{ij} + \frac{\beta_i}{\ell} (1 + k_{ex,j}) n_j \quad (19)$$

and

$$I_{im}(\Delta t) = \frac{1}{(\Delta t)^{m+1}} \int_0^{\Delta t} e^{-\lambda_i(\Delta t - \tau)} \tau^m d\tau \quad (20)$$

The solution progresses step-by-step, solving eqs. (17) and (18) simultaneously for each interval. Values of c_{ij} need not be carried along in the computation since only the values of $\dot{c}_{ij}$, which may be calculated from the equation

$$\begin{aligned}
\dot{c}_{j+1} = \dot{c}_{ij} - \lambda_i \Delta t \Big\{ & \ell \dot{c}_{ij} I_{i0}(\Delta t) + \beta_i \left[(n_j k_1 I_{i1}(\Delta t) + k_2 I_{i2}(\Delta t)) \right. \\
& + n_1 \left\{ (1 + k_{ex,j}) I_{i1}(\Delta t) + k_1 I_{i2}(\Delta t) + k_2 I_{i3}(\Delta t) \right\} \\
& + n_2 \left\{ (1 + k_{ex,j}) I_{i2}(\Delta t) + k_1 I_{i3}(\Delta t) + k_2 I_{i4}(\Delta t) \right\} \Big] \\
& \left. + \beta_i \left[n_j (k_1 + k_2) + (n_1 + n_2) (1 + k_{ex,j} + k_1 + k_2) \right] \right\} \quad , \quad (21)
\end{aligned}$$

is used in determining n_1 and n_2 .

If in any interval the excess reactivity be given as

$$k_{ex} = f(n, t) ; \quad 0 \leq t \leq \Delta t \quad , \quad (22)$$

the coefficients of the approximating curve [eq. (15)] are to be chosen so that eqs. (15) and (22) agree at the initial, end, and midpoint of the interval, i.e.,

$$k_1 = \left[-3f(n_{j,0}) + 4f \left\{ n \left(\frac{\Delta t}{2} \right), \frac{\Delta t}{2} \right\} - f \left\{ n(\Delta t), \Delta t \right\} \right] ; \quad (23)$$

$$k_2 = 2 \left[f(n_{j,0}) - 2f \left\{ n \left(\frac{\Delta t}{2} \right), \frac{\Delta t}{2} \right\} + f \left\{ n(\Delta t), \Delta t \right\} \right] . \quad (24)$$

Since $n(\frac{1}{2}\Delta t)$ and $n(\Delta t)$ are not known in the interval, they must be approximated by extrapolation from the previous interval. As a first approximation, let

$$n_1 = \Delta t \left[\frac{n_{1,j-1} + 2n_{2,j-1}}{\Delta t_{j-1}} \right] \quad (25)$$

and

$$n_2 = (\Delta t)^2 \left[\frac{n_{2,j-1}}{(\Delta t)_{j-1}^2} \right] \quad (26)$$

New values of n_1 and n_2 are then obtained from eqs. (17) and (18) by utilizing eqs. (25) and (26) in eqs. (23) and (24). Equations (17) and (18) are then solved again, using the new values of n_1 and n_2 . This iterative process is continued until

$$\left| k_{\text{ex}}^r \left(\frac{\Delta t}{2} \right) - k_{\text{ex}}^{r-1} \left(\frac{\Delta t}{2} \right) \right| + \left| k_{\text{ex}}^r(\Delta t) - k_{\text{ex}}^{r-1}(\Delta t) \right| < \epsilon \Delta t, \quad (27)$$

where ϵ is a prescribed convergence factor. The use of the Δt factor in the right-hand side of the inequality will limit accumulated errors in k_{ex} . If after a prescribed number of iterations k_{ex} has not converged, the interval size should be halved to prevent the computer getting "hung up" in a closed loop.

Upon integration of the I_{im} functions of eq. (20) for $m = 0, 1, 2, 3, 4$, there is obtained

$$I_{i0}(\Delta t) = \frac{1}{\Delta t} \left[\frac{1}{\lambda_i} \left(1 - e^{-\lambda_i \Delta t} \right) \right] \quad (28)$$

$$I_{i1}(\Delta t) = \frac{1}{(\Delta t)^2} \left[\frac{\Delta t}{\lambda_i} - \frac{1}{\lambda_i^2} \left(1 - e^{-\lambda_i \Delta t} \right) \right] \quad (29)$$

$$I_{i2}(\Delta t) = \frac{1}{(\Delta t)^3} \left[\frac{(\Delta t)^2}{\lambda_i} - \frac{2(\Delta t)}{\lambda_i^2} + \frac{2}{\lambda_i^3} \left(1 - e^{-\lambda_i \Delta t} \right) \right] \quad (30)$$

$$I_{i3}(\Delta t) = \frac{1}{(\Delta t)^4} \left[\frac{(\Delta t)^3}{\lambda_i} - \frac{3(\Delta t)^2}{\lambda_i^2} + \frac{6\Delta t}{\lambda_i^3} - \frac{6}{\lambda_i^4} \left(1 - e^{-\lambda_i \Delta t} \right) \right] \quad (31)$$

$$I_{i4}(\Delta t) = \frac{1}{(\Delta t)^5} \left[\frac{(\Delta t)^4}{\lambda_i} - \frac{4(\Delta t)^3}{\lambda_i^2} + \frac{12(\Delta t)^2}{\lambda_i^3} - \frac{24\Delta t}{\lambda_i^4} + \frac{24}{\lambda_i^5} \left(1 - e^{-\lambda_i \Delta t} \right) \right] \quad (32)$$

Evaluation of these functions maybe greatly facilitated by use of the following recurrence relation:

$$I_{i,m+1}(\Delta t) = \frac{1}{\lambda_i \Delta t} \left[1 - (m+1)I_{im} \right] \quad (33)$$

Unfortunately, if $\lambda_i \Delta t \ll 1$, the number of significant figures decreases rapidly with each application of the recursion formula. The following tables were computed for $\lambda_i \Delta t = 0.10$.

<u>Table 1</u>	<u>Table 2</u>
$I_0 = 0.95163$	$I_0 = 0.95162582$
$I_1 = 0.4837$	$I_1 = 0.4837418$
$I_2 = 0.326$	$I_2 = 0.325164$
$I_3 = 0.22$	$I_3 = 0.24508$
$I_4 = 1.2$	$I_4 = 0.1968$

Table 1 was obtained by first calculating I_0 to five significant figures and successively applying the recursion formula. Table 2 was obtained in the same fashion but starting with eight significant figures for I_0 .

Accuracy may be maintained in the cases where $\lambda_i \Delta t < 1$ by utilizing the Maclaurin expansions of the I functions:

$$I_{im} = m! \left[\frac{1}{(m+1)!} - \frac{\lambda_i \Delta t}{(m+2)!} + \frac{(\lambda_i \Delta t)^2}{(m+3)!} - \dots \right] \quad (34)$$

Computation is facilitated by first calculating I_{i4} . The maximum number of terms necessary (when $\lambda_i \Delta t \sim 1$) for an accuracy to the extent of six significant figures is six. Similarly, only eight terms of series is the maximum needed for eight-figure accuracy. The remaining functions (I_{i3} , I_{i2} , I_{i1} , I_{i0}) may then be computed with the use of the recursion relation

$$I_{im-1} = (1 - \lambda_i \Delta t I_{im})/m \quad (35)$$

The form of solution lends itself well to a method of self-checking, which will automatically change interval size as the nature of the solution requires. Rewrite eqs. (17) and (18) as

$$a_{11}(\Delta t)n_1 + a_{12}(\Delta t)n_2 = g(\Delta t) \quad (36)$$

and

$$a_{21}(\frac{1}{2}\Delta t)n_1 + a_{22}(\frac{1}{2}\Delta t)n_2 = g(\frac{1}{2}\Delta t) \quad (37)$$

An addition equation may be obtained by evaluating the basic integral equation at $\frac{1}{4}\Delta t$:

$$a_{31}(\frac{1}{4}\Delta t)n_1 + a_{32}(\frac{1}{4}\Delta t)n_2 = g(\frac{1}{4}\Delta t) \quad . \quad (38)$$

Solving eqs. (36) and (37) for n_1 and n_2 , the solution over the interval is obtained as

$$n(t) - n_j = \frac{n_1}{\Delta t} t + \frac{n_2}{(\Delta t)^2} t^2 \quad (0 \leq t \leq \Delta t) \quad . \quad (39)$$

If eqs. (37) and (38) are solved simultaneously for n_1 and n_2 , the solutions will, in general, differ somewhat, say, n_1^* and n_2^* . Thus the solution over the half-interval will be:

$$n^*(t) - n_j = \frac{n_1^*}{\Delta t} t + \frac{n_2^*}{(\Delta t)^2} t^2 \quad (0 \leq t \leq \frac{1}{2}\Delta t) \quad . \quad (40)$$

Now define

$$\epsilon(\Delta t) \equiv \left| \frac{n(\frac{1}{2}\Delta t) - n_j}{n^*(\frac{1}{2}\Delta t) - n_j} - 1 \right| = \left| \frac{n_1 + \frac{1}{2}n_2}{n_1^* + \frac{1}{2}n_2^*} - 1 \right| \quad . \quad (41)$$

If we prescribe two error bounds, ϵ_1 and ϵ_2 , to control the interval size, the three possible cases are as follows:

- I. $\epsilon_1 \leq \epsilon(\Delta t) \leq \epsilon_2 \longrightarrow$ Maintain the current interval size.
- II. $\epsilon_1 < \epsilon_2 < \epsilon(\Delta t) \longrightarrow$ Objectionable error, halve the interval size.
- III. $\epsilon(\Delta t) < \epsilon_1 < \epsilon_2 \longrightarrow$ Double the interval size for following calculations.

IV. Comparison of Methods

Example 1:

Let

$$k_{ex} = 10^{-4} \sin 0.01t \quad ; \quad (42)$$

β_i		λ_i	
0.00025	0.00241	0.01246	0.456
0.00166	0.00085	0.0315	1.612
0.00213	0.00025	0.1535	14.3

$$\begin{aligned}
S &= 0 \\
\ell &= 10^{-7} \text{ sec} \\
\Delta t &= 50 \text{ sec} \\
n(0) &= 1 \quad c_i(0) = \frac{\beta_i}{\ell \lambda_i} .
\end{aligned}$$

The fourth-order Runge-Kutta formulas are

$$n(50) = n(0) + \frac{1}{6}(k_0 + 2k_1 + 2k_2 + k_3) \quad (43)$$

and

$$c_i(50) = c_{i0} + \frac{1}{6}(m_{i0} + 2m_{i1} + 2m_{i2} + m_{i3}) \quad , \quad (44)$$

where

$$k_0 = \Delta t \dot{n}(t = 0, n_0, c_{i0}) \quad (45)$$

$$k_1 = \Delta t \dot{n}\left(\frac{1}{2}\Delta t, n_0 + \frac{1}{2}k_0, c_{i0} + \frac{1}{2}m_{i0}\right) \quad (46)$$

$$k_2 = \Delta t \dot{n}\left(\frac{1}{2}\Delta t, n_0 + \frac{1}{2}k_1, c_{i0} + \frac{1}{2}m_{i1}\right) \quad (47)$$

$$k_3 = \Delta t \dot{n}(\Delta t, n_0 + k_2, c_{i0} + m_2) \quad (48)$$

$$m_{i0} = \Delta t \dot{c}_i(t = 0, n_0, c_{i0}) \quad (49)$$

$$m_{i1} = \Delta t \dot{c}_i\left(\frac{1}{2}\Delta t, n_0 + \frac{1}{2}k_0, c_{i0} + \frac{1}{2}m_{i0}\right) \quad (50)$$

$$m_{i2} = \Delta t \dot{c}_i\left(\frac{1}{2}\Delta t, n_0 + \frac{1}{2}k_1, c_{i0} + \frac{1}{2}m_{i1}\right) \quad (51)$$

$$m_{i3} = \Delta t \dot{c}_i(\Delta t, n_0 + k_2, c_{i0} + m_{i2}) \quad . \quad (52)$$

Substitution and evaluation gives

$$\begin{aligned}
k_0 &= 0 \\
k_1 &= 12,276.8 \\
k_2 &= 23.3021 \times 10^9 \\
k_3 &= 8.742 \times 10^{16} \\
m_{i0} &= 0 \\
m_{i1} &= 247.404\beta_i \\
m_{i2} &= 3.069277 \times 10^{12} \beta_i - 6,185.1\beta_i\lambda_i .
\end{aligned}$$

Thus:

$$\underline{n(50)} = 1.457 \times 10^{16} \quad . \quad (53)$$

Using the method of RE-29, an evaluation of eq. (5) gives

$$\Delta n = \frac{(50 \times 10^7)[0 + (0.239713 \times 10^{-4})(0.998233)] - 0}{1 - (25 \times 10^7)[(0.319617 \times 10^{-4})(0.998233) - 1.760734 \times 10^{-3}]} \quad (53)$$

$$\Delta n = -3.3472 \text{ or } \underline{n(50)} = -2.3472 \quad . \quad (54)$$

Utilizing the integral equation method, the following parameters may be determined

$$\begin{aligned} k_1 &= 0.510190 \times 10^{-4} \\ k_2 &= 0.030764 \times 10^{-4} \end{aligned} \quad (55)$$

<u>m</u>	<u>$\sum_i \beta_i I_{im}(50)$</u>	<u>$\sum_i \beta_i I_{im}(25)$</u>
1	0.979149×10^{-3}	1.389685×10^{-3}
2	0.783362×10^{-3}	1.074617×10^{-3}
3	0.664719×10^{-3}	0.890789×10^{-3}
4	0.582808×10^{-3}	0.766210×10^{-3}

Equations (17) and (18) become

$$481,476 n_1 + 385,629 n_2 = 12,218 \quad (56)$$

and

$$172,672 n_1 + 66,776 n_2 = 3,116.0 \quad (57)$$

Solving eqs. (56) and (57),

$$n = 1 + 0.011201 \left(\frac{t}{50}\right) + 0.017698 \left(\frac{t}{50}\right)^2 ; \quad 0 \leq t \leq 50 \quad (58)$$

$$\underline{n(50)} = 1.028899 \quad (59)$$

The example was also solved by the integral equation method in two steps. The resulting values were:

$$n(25) = 1.010290 \quad (60)$$

$$\underline{n(50)} = 1.028777 \quad (61)$$

Example II

Let

$$\left. \begin{aligned} k_{ex} &= 0.755t \text{ (\$100/sec)} \\ \Delta t &= 0.001 \text{ sec} \end{aligned} \right\} , \quad (62)$$

the other parameters being the same as in Example I.

The Runge-Kutta method is as useless here as in the previous example:

$$\begin{aligned} k_0 &= 0 \\ k_1 &= 3.746 \\ k_2 &= 130.665 \\ k_3 &= 8962 \\ \underline{n(0.001)} &= 1452 \end{aligned} \quad (63)$$

Solutions for this example were obtained by means of the RE-129 code with the IBM-704 for several interval sizes:

$$\Delta t = 10^{-3} \text{ (1 step),} \quad \underline{n(0.001)} = 1.10339 \quad (64)$$

$$\Delta t = 10^{-4} \text{ (10 steps),} \quad \underline{n(0.001)} = 1.10842 \quad (65)$$

$$\Delta t = 10^{-5} \text{ (100 steps),} \quad \underline{n(0.001)} = 1.10844 \quad (66)$$

The integral equation method for a single step ($\Delta t = 0.001$) yielded:

$$36.24164 n_1 + 24.28802 n_2 = 3.746507 \quad (67)$$

$$9.623951 n_1 + 3.278417 n_2 = 0.936626 \quad (68)$$

$$n_1 = 0.091107$$

$$n_2 = 0.018308$$

$$\underline{n(0.001)} = 1.109415 \quad (69)$$