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NUMERICAL INTEGRATION
OF DYNAMIC NUCLEAR SYSTEMS EQUATIONS
BY OPTIMUM INTEGRATING FACTORS

by

Phillip Allen Secker, Jr.

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I hereby recommend that this dissertation prepared under my direction by PHILLIP ALLEN SECKER, JR.

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ABSTRACT

The numerical integration of the ordinary, nonlinear, differential equations of nuclear reactor kinetics has been the subject of much investigation. In this work a new numerical method called the method of optimum integrating factors is presented. The method is developed from a special integral equation solution of a first order ordinary differential equation. An integrating factor is formulated whose exponent is complex. By expansion of the integrand of the integral equation in Taylor series, a series approximation to the variable of integration is obtained which constitutes the basic numerical method.

The advantages of the numerical method proposed are several. Other numerical techniques based on an integral equation formulation have proven to be extremely well suited to solving reactor kinetics problems using large integration steps, and this method also possesses this quality. Since an approximating series of arbitrary order N is used, an analytic expression for the truncation error may be obtained. An equation for automatically determining the integration step size is achieved by requiring that the relative truncation error be no greater than a prescribed criterion. Further, the integration step size may be maximized by properly computing

the real and imaginary parts of the integrating factor exponent. The theory predicts that these parameters are only functions of the behavior of the dependent variable of integration. Programming the method on a digital computer proved to be straightforward.

The method of optimum integrating factors was used to obtain approximate solutions to three first order prompt neutron kinetics problems for which analytic solutions are known. The agreement between the approximate and the analytic solutions is excellent. Nowhere do local solution errors exceed the error criteria.

Delayed neutron kinetics studies were made for problems where analytic solutions are not known. The merits of using a complex integrating factor exponent were verified for these higher order problems. Comparisons were made of solution computational times using optimum integrating factors and other numerical integration techniques. In all cases the present method was the fastest. The solutions obtained agreed closely with those computed by the other methods and with predicted approximations.

It was concluded that the method of optimum integrating factors is a powerful technique for solving the dynamic equations of nuclear systems. Significant increases in the integration step size were possible using complex inverse time constants.

CHAPTER 1

INTRODUCTION

This study presents a numerical integration algorithm derived from an integral equation formulation for the general solution of first order (including nonlinear) ordinary differential equations. The method, although general enough for the numerical solution of any set of ordinary differential equations, is specifically applied to the numerical solution of the space- and energy-independent reactor kinetics equations. The integral equation of this method results from the selection of an integrating factor whose exponent is complex.

The numerical solution of the reactor kinetics equations has been the subject of a considerable amount of research in the last decade. The problem is that generally the time constant associated with neutron population changes is exceedingly small compared to those associated with other competing dynamic effects. The numerical solution of slow transients in nuclear reactors using any of the various finite difference techniques is sometimes a prohibitively time consuming task, even for modern computers.

The concept of using an integral equation for the basis of numerical integration methods has become a very powerful approach for increasing the numerical integration step size. Integrating factors with pure real exponents have been successfully used in numerical integration methods with excellent results in solving some nuclear reactor kinetics problems[1,4]. Many classes of ordinary differential equations (linear, non-linear and/or parameter varying), however, cannot be efficiently solved by such methods. Even reactor kinetics equations, when coupled to equations of heat transfer, coolant dynamics, or control mechanisms, may not always be solved efficiently by such a method. Some of the limitations will become clear.

Existing numerical integration techniques all exhibit a number of disadvantages. In the search for a single integration method appropriate for solving any set of differential equations, regardless of driving force amplitudes and/or time constants, minimization of the various disadvantages was attempted in the method proposed here. Hence-forth this method is called the method of "optimum integrating factors." Some of the limitations inherent in other numerical methods are itemized.

1. Stability of some methods, such as finite difference techniques, limit the maximum permissible integration step size. These integration techniques[8,15], in general, approximate the integrating factor with various order approximations. The integration step size then

is limited by the smallest time constant of the system. In contrast the integration step size for the method of optimum integration factors is dependent on the solution response characteristics.

2. Integral equation techniques, such as the method of Adler and Cohen[1,4] which approximate the slowly-varying factors in the integrands, use arbitrary standards in the selection of inverse time constants for the exponent of the integrating factors. The method of optimum integrating factors, however, uses an analytic criterion in the selection of these parameters which maximizes the integration step size at every point in the solution.

3. Some methods are based on a matrix formulation of the differential equation system. Hansen's method[9] and Porsching's method[16] are examples of techniques which formulate the integral equation on a matrix basis. A disadvantage of such a method is that as the order of the differential equation system increases the number of computer computations increases in the ratio at least proportional to the square of the number of equations. Computational times using the method of optimum integrating factors increase only linearly with the increase in the number of differential equations since a single scalar equation is appropriate for the solution of each differential equation.

4. Some methods require special equation formulation. Collocation techniques such as those developed by Brittan[3],

Kaganove[11], or Flatt[7] exhibit this feature. The Laplace transform technique of Keepin and Cox[12] also suffers in this respect. Considerable success has been achieved with these methods when solving the basic point reactor kinetics equations with reactivity treated as an input. However, the task of manipulating the equations for high order system or nonlinear systems can be almost insurmountable. The formulation of the method of optimum integrating factors is such that each equation be formulated as a first order ordinary differential equation. Therefore any dynamic system, regardless of its order or degree of nonlinearity, can be handled in its full generality very simply.

Additionally, most methods, including those already cited, suffer from the following limitations.

1. No analytic criterion exists for the computation of the integration step size.

2. Arbitrary criteria are used in changing the integration step size during the solution.

3. Some methods are not self-starting.

4. The magnitude of the local error is neither known nor analytically controllable.

The method of continuous analytic continuation developed by Vigil[20] was the first method to circumvent all of these limitations. The method of optimum integrating factors parallels Vigil's method in all of these respects. In addition, the method of optimum integrating factors is based on an integral equation approach and thus combines the advantages of Vigil's method and integral equation methods.

The method proposed was sucessfully written into a digital computer subroutine to solve any completely general set of differential equation systems. All of the nuclear reactor dynamic problems presented in this work were programmed as individual problems as would be done with any other type of dynamic system. In most cases studied it was considered desirable to make comparisons of the method of optimum integrating factors with some other numerical method. Comparisons were made of computer running times and solution accuracy with the method of continuous analytic continuation for a number of cases for which analytic solutions exists.

Combining the best features of many of the more powerful numerical integration techniques gives a single method which is optimum in several respects. Results presented herein verify that the method is competitive with all of the techniques now in use.

CHAPTER 2

OPTIMUM INTEGRATING FACTORS

The method of optimum integrating factors is developed from a basic integral equation solution of an ordinary first order differential equation. Derivations of the method and analytic criteria for maximizing the integrating step size and controlling the local error are given in this chapter.

The Integral Equation

An integral equation can be proposed for the general solution of the first order ordinary differential equation

$$dy(t)/dt = f[y(t),t] \tag{2.1}$$

by choosing an integrating factor whose exponent is complex. To do so, equation (2.1) is modified to

$$dy(t)/dt = -(\alpha + i\beta)y(t) + (\alpha + i\beta)y(t) + f[y(t),t] \tag{2.2}$$

where α and β are the inverse time constant magnitudes of the real and imaginary parts, respectively, of the integrating factor exponent; $i = \sqrt{-1}$. The integral equation solution of $y(t)$ at $t_{j+1} = t_j + \Delta t$, where t_j is the initial value of the independent variable t, using the integrating factor $\exp[-(\alpha + i\beta)\Delta t]$, is

$$y(t_{j+1}) = y(t_j) \exp[-(\alpha + i\beta)\Delta t] + \exp[-(\alpha + i\beta)\Delta t]$$

$$\times \int_0^{\Delta t} \left| (\alpha + i\beta) y(t_j + \tau) + f\left[y(t_j + \tau), t_j + \tau\right] \right|$$

$$\times \exp[(\alpha + i\beta)\tau] d\tau \tag{2.3}$$

where Δt is the integration step size.

Using the familiar Euler relations

$$\exp(+i\beta x) = \cos \beta x + i \sin \beta x \tag{2.4}$$

and

$$\exp(-i\beta x) = \cos \beta x - i \sin \beta x , \tag{2.5}$$

equation (2.3) can be rewritten in terms of sine and cosine functions. The resulting integral equation consists of a real and an imaginary component. Without difficulty it can be demonstrated that the imaginary part of the solution is identically zero (see Appendix A). The real part of the solution, the portion of interest, is

$$y(t_{j+1}) = y(t_j) \exp(-\alpha \Delta t) \cos \beta \Delta t$$

$$+ \exp(-\alpha \Delta t) \int_0^{\Delta t} \left| \alpha y(t_j + \tau) + f\left[y(t_j + \tau), t_j + \tau\right] \right|$$

$$\times \cos \beta(\tau - \Delta t) \exp(\alpha \tau) d\tau - \exp(-\alpha \Delta t) \int_0^{\Delta t} \beta y(t_j + \tau)$$

$$\times \sin \beta(\tau - \Delta t) \exp(\alpha \tau) d\tau . \tag{2.6}$$

Equation (2.6) is the fundamental integral equation from which the numerical integration method of optimum integrating factors is derived. Validity of equation (2.6) is independent of the values of α and β. The evaluation of the two integrals of equation (2.6) is complicated by the fact that y(t) and f[y(t),t] are not generally analytic functions of the independent variable t. Note that if β is zero, equation (2.6) reduces to the integral equation on which the method of Adler and Cohen is based.

The Numerical Method

It is impossible, generally, to obtain closed form (analytic) solutions to equation (2.6). Evaluation of the two integrals may be approximated therefore by applying numerical techniques. The approximation chosen in the derivation of the method of optimum integrating factors consists of expanding the dependent variables y(t) and f[y(t),t] in Taylor series. Since a Taylor series may be truncated after any number of terms desired, an infinite number of approximations to the solution could be derived. For the proposed method, terms beyond the third derivative in y(t), namely $y^{(3)}(t)$, have been eliminated for the evaluation.

The theory of complex variables [14] specifies that in order to expand a dependent variable in a Taylor series the variable must be regular or analytic in the region of expansion. Complex dependent variables which exhibit singular points

(points at which discontinuities in their derivatives exist) may be treated using a Taylor series. Successive regions of integration are chosen which neither intersect nor enclose any of the singular points. This is known as continuous analytic continuation.

However, the dependent variables of the systems of differential equations generally encountered in reactor kinetics studies are functions of the real independent variable t only. Therefore the path of integration is confined to the real axis and singular points cannot be avoided. Thus, if a singularity is encountered in a dependent variable at t_s, the integration step size Δt must be limited such that

$$t_j + \Delta t \leq t_s \ .$$

The solution may be continued beyond t_s using Taylor series by reevaluating all derivatives at t_s^+.

The Taylor series representation for $y(t_j + \tau)$ which is used in equation (2.6) is

$$y(t_j + \tau) = \sum_{k=o}^{N} y^{(k)}(t_j)\tau^k/(k!) \ . \qquad (2.7)$$

In this equation, $y^{(k)}(t_j)$ represents the k^{th} derivative of $y(t)$ evaluated at $t = t_j$. The Taylor series expansion of $y(t_j + \tau)$ has been carried to order N.

The basic numerical integration equation results by substituting equation (2.7) into the integrals of equation (2.6).

$$y(t_{j+1}) = y(t_j)\exp(-\alpha\Delta t)\cos\beta\Delta t$$

$$+ \exp(-\alpha\Delta t)\sum_{k=o}^{N}\int_o^{\Delta t}\left[\alpha y^{(k)}(t_j) + y^{(k+1)}(t_j)\right]$$

$$\times \frac{\tau^k}{(k!)}\cos\beta(\tau - \Delta t)\exp(\alpha\tau)d\tau - \exp(-\alpha\Delta t)$$

$$\times \sum_{k=o}^{N}\int_o^{\Delta t}\beta y^{(k)}(t_j)\frac{\tau^k}{(k!)}\sin\beta(\tau - \Delta t)\exp(\alpha\tau)d\tau \ . \tag{2.8}$$

This equation may be further reduced by employing the following trigonometric identities:

$$\cos\beta(\tau - \Delta t) = \cos\beta\tau\cos\beta\Delta t + \sin\beta\tau\sin\beta\Delta t$$

$$\sin\beta(\tau - \Delta t) = \sin\beta\tau\cos\beta\Delta t - \cos\beta\tau\sin\beta\Delta t \ .$$

After substitution of these identities into equation (2.8) one is left with the evaluation of the following fundamental integral functions:

$$Ic_{m+1}(x) = \frac{e^{-\alpha x}}{m!}\int_o^x \tau^m e^{\alpha\tau}\cos\beta\tau d\tau$$

and

$$Is_{m+1}(x) = \frac{e^{-\alpha x}}{m!}\int_o^x \tau^m e^{\alpha\tau} \sin \beta\tau d\tau \ .$$

Evaluation of these integrals is performed in Appendix B and recursive relationships have been derived. They are

$$Ic_{m+1}(x) = \frac{x^m}{m!}\left[\frac{\alpha \cos \beta x + \beta \sin \beta x}{\alpha^2 + \beta^2}\right] - \frac{\alpha Ic_m(x)}{\alpha^2 + \beta^2} - \frac{\beta Is_m(x)}{\alpha^2 + \beta^2}$$

$$Is_{m+1}(x) = \frac{x^m}{m!}\left[\frac{\alpha \sin \beta x - \beta \cos \beta x}{\alpha^2 + \beta^2}\right] - \frac{\alpha Is_m(x)}{\alpha^2 + \beta^2} + \frac{\beta Ic_m(x)}{\alpha^2 + \beta^2}$$

where

$$Ic_1(x) = \frac{\alpha \cos \beta x + \beta \sin \beta x - \alpha e^{-\alpha x}}{\alpha^2 + \beta^2}$$

and

$$Is_1(x) = \frac{\alpha \sin \beta x - \beta \cos \beta x + \beta e^{-\alpha x}}{\alpha^2 + \beta^2}$$

In the event that α exists and β is zero the functions $Is_m(x)$ are identically zero and the functions $Ic_m(x)$ reduce to the so-called $C_m(x)$ and $H_m(x)$ functions[4,10]. These functions are required in the method of Adler and Cohen since they have chosen to use an integrating factor with a pure real exponent.

The result of substituting the above identities into equation (2.8) yields a numerical approximation to $y(t_{j+1})$ which is considerably more simple.

$$y(t_{j+1}) = \sum_{k=o}^{N-1} y^{(k)}(t_j)\Delta t^k/(k!) + F_N(\alpha,\beta,\Delta t)y^{(N)}(t_j) \qquad (2.9)$$

This numerical algorithm closely resembles a Taylor series except for the final term. In fact if α and β are identically zero equation (2.9) becomes a Taylor series approximation of order N. The coefficient F_N is determined from the equation

$$F_N(\alpha,\beta,\Delta t) = Ic_N(\Delta t)\cos\beta\Delta t + Is_N(\Delta t)\sin\beta\Delta t\ . \qquad (2.10)$$

Equation (2.9) may be easily programmed on a digital computer. As a foundation for a numerical method this equation possesses several advantages. The technique is self-starting for a system of first order differential equations requiring only the initial conditions on the dependent variables at $t = 0+$. The values of the derivatives of $y(0+)$ may be obtained by successive differentiation of the differential equations. Equation (2.9) never increases in complexity but remains the same for every integration interval. During each integration interval the solution of $y(t_{j+1})$ is obtained from the value of the dependent variable and its derivative at t_j only. Some numerical methods require a knowledge of the values of the dependent variables at several preceding points.

In order to solve for $y(t_{j+1})$ using equation (2.9) a number of problems must still be resolved. At this point the values of α, β, and Δt must be specified. For most numerical methods the value of Δt is arbitrarily selected on the basis of a priori information or experience. An analytic criterion for determination of the integration step size has been developed for this method. The selection of α in the method of

Adler and Cohen is also arbitrary. The values of α and β for this method are computed at each point of the solution such that Δt is maximized; hence the name optimum integrating factors.

Analytic Criterion for the Integration Step Size

The basic numerical integration equation, equation (2.9), is a power series of order N. By requiring that the magnitude of the relative truncation error of the series always be at most equal to a specified error criterion an expression for Δt can be obtained.

The remainder of the truncated power series after N+1 terms is obtained by subtracting the N^{th} order series from an $(N+1)^{st}$ order series. The result is (in Lagrangian [5] form)

$$R_N(t_{j+1}) = y^{(N)}(\eta)\left[\frac{\Delta t^N}{N!} - F_N\right] + y^{(N+1)}(\eta)F_{N+1} \tag{2.11}$$

where $t_j \leq \eta \leq t_{j+1}$,

and

$$\begin{aligned} y^{(m)}(\eta) &= \int_{t_j}^{t_{j+1}} y^{(m)}(t)\,dt/(t_{j+1} - t_j) \\ &= \left[y^{(m-1)}(t_{j+1}) - y^{(m-1)}(t_j)\right]/(t_{j+1} - t_j) \\ &= \delta y^{(m-1)}/\Delta t. \end{aligned} \tag{2.12}$$

The equation for the relative truncation error is merely the absolute value of the remainder divided by the dependent variable at t_{j+1}.

$$\left| R_N(t_{j+1})/y(t_{j+1}) \right| \leq \epsilon \ . \tag{2.13}$$

Using equation (2.12), $R_N(t_{j+1})$ becomes

$$R_N(t_{j+1}) = \left[\delta y^{(N-1)} \left(\frac{\Delta t^N}{N!} - F_N \right) + F_{N+1} \delta y^{(N)} \right] / \Delta t. \tag{2.14}$$

The coefficients F_N and F_{N+1} are given by equation (2.10). In Appendix C it is demonstrated that equation (2.10) may be rewritten as

$$F_N = \sum_{k=o}^{\infty} \frac{c_k \Delta t^{N+k}}{(N+k)!} \tag{2.15}$$

where c_k are coefficients of the series for exp $(-\alpha\Delta t)$ cos $\beta\Delta t$ which is

$$\exp(-\alpha\Delta t) \cos \beta\Delta t = \sum_{k=o}^{\infty} \frac{c_k \Delta t^k}{k!} \ .$$

Recursion formulae have been developed for c_k in terms of s_k, the coefficients of the series for exp $(-\alpha\Delta t)$ sin $\beta\Delta t$, which is

$$\exp(-\alpha\Delta t)\sin\beta\Delta t = \sum_{k=o}^{\infty} \frac{s_k \Delta t^k}{k!} .$$

These recursion formulae are

$$c_{k+1} = -\alpha c_k - \beta s_k$$

and

$$s_{k+1} = \beta c_k - \alpha s_k$$

where $c_o = 1$ and $s_o = 0$. Some additional properties of c_k and s_k are noted in the following relationships:

$$c_{k+\ell} = c_k c_\ell - s_k s_\ell$$

$$s_{k+\ell} = c_k s_\ell + s_k c_\ell$$

and
$$c_k^{\,2} + s_k^{\,2} = (\alpha^2 + \beta^2)^k .$$

Table I lists the first 6 coefficients for the two series.

The remainder $R_N(t_{j+1})$, after substitution of equation (2.15), can now be written

$$R_N(t_{j+1}) = \sum_{k=o}^{\infty} \frac{\Delta t^{N+k}}{(N+k+1)!}\left[c_k \delta y^{(N)} - c_{k+1}\delta y^{(N-1)}\right] . \qquad (2.16)$$

The relative truncation error of equation (2.13) becomes a nonlinear polynomial equation in Δt.

TABLE I

Coefficients of the Decaying Cosinusoidal and Sinusoidal Series

$$\text{I.A} \quad \exp(-\alpha\Delta t)\cos\beta\Delta t = \sum_{i=o}^{\infty} c_i \Delta t^i / i!$$

$c_0 = 1$

$c_1 = -\alpha$

$c_2 = \alpha^2 - \beta^2$

$c_3 = -\alpha^3 + 3\alpha\beta^2$

$c_4 = \alpha^4 - 6\alpha^2\beta^2 + \beta^4$

$c_5 = -\alpha^5 + 10\alpha^3\beta^2 - 5\alpha\beta^4$

$c_6 = \alpha^6 - 15\alpha^4\beta^2 + 15\alpha^2\beta^4 - \beta^6$

$$\text{I.B} \quad \exp(-\alpha\Delta t)\sin\beta\Delta t = \sum_{i=o}^{\infty} s_i \Delta t^i / i!$$

$s_0 = 0$

$s_1 = \beta$

$s_2 = -2\alpha\beta$

$s_3 = -\beta^3 + 3\alpha^2\beta$

$s_4 = 4\alpha\beta^3 - 4\alpha^3\beta$

$s_5 = \beta^5 - 10\alpha^2\beta^3 + 5\alpha^4\beta$

$s_6 = -6\alpha\beta^5 + 20\beta^3\beta^3 - 6\alpha^5\beta$

$$\sum_{k=o}^{\infty} \frac{\Delta t^{N+k}}{(N+k+1)!} \left| \frac{c_k \delta y^{(N)} - c_{k+1} \delta y^{(N-1)}}{y(t_{j+1})} \right| \leq \epsilon \ . \tag{2.17}$$

It is demonstrated in Appendix D, using the relative error equation for the power series of order (N-1), that the term within the absolute value sign can be expressed as

$$c_k \delta y^{(N)} - c_{k+1} \delta y^{(N-1)} = c_k \left[(c_1{}^2 + s_1{}^2) \delta y^{(N-2)} - 2c_1 \delta y^{(N-1)} + \delta y^{(N)} \right] \tag{2.18}$$

to a first approximation. The relative truncation error may now be expressed as

$$\left| \frac{(c_1{}^2 + s_1{}^2) \delta y^{(N-2)} - 2c_1 \delta y^{(N-1)} + \delta y^{(N)}}{y(t_{j+1})} \right| \sum_{k=o}^{\infty} \frac{c_k \Delta t^{N+k}}{(N+k+1)!} \leq \epsilon \ . \tag{2.19}$$

The infinite summation in equation (2.19) may be reduced to the following inequality:

$$\sum_{k=o}^{\infty} \frac{c_k \Delta t^{N+k}}{(N+k+1)!} \leq \frac{\Delta t^N}{(N+1)!} \left[\frac{1}{1 - \frac{2c_1 \Delta t}{(N+2)} + \frac{(c_1{}^2 + s_1{}^2) \Delta t^2}{(N+2)(N+3)}} \right] . \tag{2.20}$$

Finally, an analytic criterion for computing Δt has been determined after substituting equation (2.20) into equation (2.19) and setting the result equal to ϵ.

$$\Delta t = \left\{ \frac{(N+1)!\,\epsilon \left| y(t_{j+1}) \right| \left[1 - \frac{2c_1 \Delta t}{(N+2)} + \frac{(c_1{}^2 + s_1{}^2)\Delta t^2}{(N+2)(N+3)} \right]}{\left| (c_1{}^2 + s_1{}^2)\delta y^{(N-2)} - 2c_1 \delta y^{(N-1)} + \delta y^{(N)} \right|} \right\}^{1/N} \qquad (2.21)$$

The integration step size, therefore, is determined by the error criterion ϵ, the order N of the series expansion, the behavior of y(t) in the interval $t_j \le t \le t_{j+1}$, and the values of α and β. It is significant that when N and ϵ are fixed, the integration step size is largest where y(t) varies the least; smallest where y(t) varies the most rapidly. The analytic criterion, therefore, provides automatic (adaptive) expansion and contraction of Δt depending only on the behavior of y(t) limiting the relative local error to ϵ.

For a system of M first order differential equations equation (2.21) must be computed for each of the M dependent variables. The integration process requires a common integration step size for all of the M variables. Therefore, using the smallest Δt computed guarantees that the error in every variable never exceeds the specified error criterion of equation (2.13).

Note that in the equation for Δt the right hand side contains terms in Δt. In the practical evaluation of equation (2.21), experience has shown that using Δt from the prior integration interval on the right hand side is always satisfactory and considerably reduces the computation effort. Since Δt is determined from the N^{th} root of the right hand expression it is not a sensitive function of the defining parameters.

Maximizing the Integration Step Size

The values of α and β throughout the development of the basic numerical method and the analytic criterion for Δt have not been specified. Actually all of the preceding development is completely valid regardless of their values. The primary reason, however, for going to such lengths to develop an integration technique using complex inverse time constants was to significantly increase the integration step size depending on the behavior of y(t). It is obviously desirable to use the maximum permissible integration step size for any digital computer integration technique.

Observing equation (2.21) it is noted that, in order to maximize Δt, the following relationship holds:

$$(\alpha^2 + \beta^2)\delta y^{(N-2)} + 2\alpha\delta y^{(N-1)} + \delta y^{(N)} = 0$$

where $c_1 = -\alpha$ and $s_1 = \beta$. This is a single equation with two unknowns, namely α and β. If the series were only of the order N-1, however, the condition for maximizing Δt for this series is

$$(\alpha^2 + \beta^2)\delta y^{(N-3)} + 2\alpha\delta y^{(N-2)} + \delta y^{(N-1)} = 0.$$

Upon combining these two relationships, the equations required to evaluate α and β can be determined. An alternate way of computing α and β is obtained by introducing the definitions

$$\omega^2 \equiv \alpha^2 + \beta^2$$

and

$$\alpha \equiv \omega\zeta \ .$$

For the most general second order linear ordinary differential equation ω represents the natural frequency of the solution and ζ represents the damping ratio. Substituting and solving for ω and ζ the following relationships are obtained:

$$\omega^2 = \frac{\delta y^{(N)}\delta y^{(N-2)} - \delta y^{(N-1)}\delta y^{(N-1)}}{\delta y^{(N-1)}\delta y^{(N-3)} - \delta y^{(N-2)}\delta y^{(N-2)}} \tag{2.22}$$

$$\zeta = -\left[\frac{\delta y^{(N)} + \omega^2\delta y^{(N-2)}}{2\omega\delta y^{(N-1)}}\right]. \tag{2.23}$$

Utilizing the preceding definitions, the values of α and β which maximize Δt are now obtainable. These parameters are seen to be only functions of the behavior of y(t) in the integration interval.

The numerical method has been formulated for a series of arbitrary order N. Observing equation (2.22) it is noted that in order to evaluate α and β optimally one is required to generate at least $\delta y^{(N-3)}$, $\delta y^{(N-2)}$, $\delta y^{(N-1)}$ and $\delta y^{(N)}$. The lowest value of N, therefore, that must be specified is N = 3. For this reason the 3rd order power series has been used throughout this work to obtain results. This requires that $y(t)$ and its first three derivatives be programmed for the solution.

Initially it was felt that the derivatives of $y(t)$ greater than $y^{(1)}(t)$ might be obtained numerically from the solution. It is well documented, however, that numerical differentiation is sometimes orders of magnitude less accurate than numerical integration[15]. The problem arises from the fact that there may be extreme magnitude differences in the values of $y(t)$ and $y^{(1)}(t)$. In other words, it is easier to predict numerically an area than the slope of a line using prior data. Since prior data would be required, special starting techniques would be necessary. Experience has shown that when $y^{(2)}(t)$ and $y^{(3)}(t)$ were numerically evaluated the method of optimum integrating factors was numerically unstable.

Without the physical understanding of second order linear differential equations one might be tempted to use directly the values of α and β obtained from equations (2.22) and (2.23). Under certain conditions imaginary values of β may be obtained. This means that the exponent of the integrating factor, which was chosen to be complex, in truth is real only.

A summary of the particular conditions which can occur follows. Four basic equations for each situation are specified corresponding to the equations for $F_N(\alpha,\beta,\Delta t)$, Δt, α and β.

1. When the solution is stationary, or steady state conditions have been achieved, all derivatives will be zero and

$$\omega^2 = 0.$$

In this situation $\alpha = \beta = 0$.

The equation for F_N is

$$F_N = \frac{\Delta t^N}{N!},$$

and the analytic equation for Δt is

$$\Delta t = \left\{ \frac{(N+1)!\,\epsilon \left| y(t_{j+1}) \right|}{\left| \delta y^{(N)} \right|} \right\}^{1/N}.$$

Under these conditions a pure Taylor series approximation is used in computing $y(t_{j+1})$. This is precisely the format for the method of continuous analytic continuation[20]. It should be noted, however, that if the solution is non-stationary there are always values for either α or β or both. Also if the solution is stationary the predicted value of Δt is infinity.

The values of α and β are generated on the basis of the solution behavior during Δt. This behavior is unknown until at least one integration interval has been traversed; therefore, the Taylor series is an effective starting procedure.

2. Occasionally a portion of the solution may behave like an undamped sinusoid (cosinusoid). The situation is

$$\zeta = 0.$$

Thus

$$\alpha = 0$$

and

$$\beta^2 = -\delta y^{(N)}/\delta y^{(N-2)} .$$

F_N is evaluated as

$$F_N = \mathrm{Re}\left\{\left[\cos \beta\Delta t - i \sin \beta\Delta t - \sum_{k=o}^{N-1} \frac{(-i\beta\Delta t)^k}{k!}\right] \Big/ (-i\beta)^N\right\} ,$$

and the analytic criterion for Δt is

$$\Delta t = \left\{ \frac{(n+1)!\epsilon \left| y(t_{j+1}) \right| \left[1 + \dfrac{\beta^2 \Delta t^2}{(N+2)(N+3)}\right]}{\left| \beta^2 \delta y^{(N-2)} + \delta y^{(N)} \right|} \right\}^{1/N} .$$

3. If the magnitude of the absolute value of ζ is greater than unity critical damping is exceeded. The solution bears no resemblance to sinusoidal behavior.

For

$$|\zeta| > 1$$

$$\alpha = -\delta y^{(N)}/\delta y^{(N+1)} ,$$

$$\beta = 0,$$

$$\Delta t = \left\{ \frac{(N+1)!\,\epsilon \left| y(t_{j+1}) \right| \left[1 + \alpha\Delta t/(N+2) \right]}{\left| \alpha\delta y^{(N-1)} + \delta y^{(N)} \right|} \right\}^{1/N} ;$$

and

$$F_N = \left[\exp\,(-\alpha\Delta t) - \sum_{k=o}^{N-1} \frac{(-\alpha\Delta t)^k}{k!} \right] \Big/ (-\alpha)^N$$

The series which results in this situation is analagous to the method of Adler and Cohen.

4. Finally the relationships of optimum integrating factors apply in their full generality when

$$\omega^2 > 0$$

and

$$-1 \le \zeta \le 1.$$

In this case β is always non-negative and α assumes the sign of ζ. Restating the equations for α, β, F_N and Δt,

$$\alpha = \omega\zeta$$

$$\beta = \sqrt{\omega^2 - \alpha^2}$$

$$F_N = \frac{\exp\,(-\alpha\Delta t)}{\omega^{2N}} \left[c_N \cos \beta\Delta t + s_N \sin \beta\Delta t \right] - \sum_{k=1}^{N} \frac{c_k \Delta t^{N-k}}{\omega^{2k}(N-k)!}$$

$$\Delta t = \left\{ \frac{(N+1)!\,\epsilon\,\left|y(t_{j+1})\right| \left[1 + \frac{2\omega\zeta\Delta t}{(N+2)} + \frac{\omega^2\Delta t^2}{(N+2)(N+3)}\right]}{\left|\omega^2\delta y^{(N-2)} + 2\omega\zeta\delta y^{(N-1)} + \delta y^{(N)}\right|} \right\}^{1/N}$$

Programming the Method

The equations associated with the method of optimum integrating factors were coded into a digital computer integration subroutine. This subroutine was used in the TAF (Time and Frequency) digital simulation program[17] for all of the studies in this work. The TAF code is used to study the behavior of any system that can be represented by a group of first order nonlinear ordinary differential equations. The user, therefore, is not restricted to the solution of reactor kinetics equations only.

Two user coded subroutines are required to define the input parameters and the derivatives of the system under study. The method of optimum integrating factors requires 10 computer storage locations for each of the M differential equations in an M^{th} order problem. These storage locations correspond to:

1. $y(t_j)$	6. $y^{(2)}(t_{j+1})$
2. $y(t_{j+1})$	7. $y^{(3)}(t_j)$
3. $y^{(1)}(t_j)$	8. $y^{(3)}(t_{j+1})$
4. $y^{(1)}(t_{j+1})$	9. $\alpha(t_j)$
5. $y^{(2)}(t_j)$	10. $\beta(t_j)$

These are the variables required if the order N of the approximation to $y(t_{j+1})$ is equal to 3. For any higher order approximation two additional storage variables are required per derivative.

The method is self-starting; however, α and β cannot be computed until at least one Δt interval has been traversed. For this reason, a simple Taylor series starts the integration process. An option has been coded whereby the computation of α and β is suppressed. The resulting algorithm is that of continuous analytic continuation. For the studies presented in Chapter 3, this option was exercised in each case in order to compare the accuracy and computational times to those obtained using optimum integrating factors.

The integration step size used for the starting value is initially determined within the subroutine. It is determined numerically by computing the system time constants at $t = 0^+$ and setting

$$\Delta t = |\tau_{min}|$$

where τ_{min} is the smallest system time constant. For the neutron kinetics equations this value, for small values of reactivity, is very nearly equal to the neutron generation time, ℓ, divided by the total fraction of delayed fission neutrons, β_{eff}:

$$\Delta t \approx \ell / \beta_{eff} .$$

For large positive values of reactivity, the largest negative eigenvalue decreases and the initial Δt need not be so small.

After making an initial pass through all of the derivative equations, values for $y(t_{j+1})$ and its derivatives are predicted. A new value for Δt is computed from the analytic criterion for the integration step size. If this new Δt is greater than the initial value (or very slightly smaller) the integration proceeds. Otherwise this new value of Δt becomes the initial integration step and a new approximation for $y(t_{j+1})$ is calculated. This iteration process continues until the error criterion on all system variables is satisfied. Experience has shown that seldom are more than two such iterations necessary. Frequently the initial Δt is sufficient.

It has been determined that values of the relative error criterion ϵ in the range

$$10^{-6} \leq \epsilon \leq 10^{-3}$$

guarantee fewer iterations at each step and, consequently, lower computer running times. Values of ϵ less than 10^{-6} increase the number of time steps significantly to achieve what may be unreasonable accuracy. Values of ϵ greater than 10^{-3} sometimes cause an excessive number of iterations at certain points in the solution. This is frequently the case where the solution exhibits large changes. Large values of ϵ yield large values of Δt, whereas large changes in $y(t)$ yield smaller values of Δt; the incompatibility of these two conditions requires many iterations and longer computational times. A limit of 5 iterations at each t_{j+1} is imposed in the subroutine to prevent such problems. This limit has not been exceeded in any of the reactor kinetics problems where ϵ was less than 10^{-3}.

When any of the dependent variables have zero initial conditions or become zero during their solution the predicted Δt is zero. When this condition arises the Δt of the prior integration interval is used.

CHAPTER 3

RESULTS

The method of optimum integrating factors was applied to the solution of various reactor neutron kinetics problems. A number of first order prompt neutron kinetics problems for which analytic solutions exist were studied and clearly illustrate the advantages of optimum integrating factors.

Comparisons of accuracy and computer running times were made in most problems using the methods of optimum integrating factors and continuous analytic continuation. Computer running times using optimum integrating factors were shorter for all of the problems studied. When problems with analytic solutions were solved, the accuracy achieved using optimum integrating factors was always superior to that obtained with continuous analytic continuation.

Higher-than-first order problems were investigated to illustrate the advantages of using complex inverse time constants. To demonstrate this advantage these problems were solved using both complex and real (only) inverse time constants. The latter was accomplished by suppressing the computation of β, the imaginary component of this complex parameter.

The Neutron Kinetics Equations

The reactor neutron kinetics equations are fundamental relationships which describe the dynamics of neutron population changes within any nuclear reactor. These equations can be derived from the time-dependent Boltzmann transport equation for neutrons in stationary reactor systems[22]. The basic assumption made in this derivation is that the neutron behavior is aptly described using space-, energy-, and direction-averaged equations.

Two variations of the neutron kinetics equations are studied here. First, prompt neutron kinetics are considered where it is assumed that none of the neutrons released during the fission process is delayed. Second, delayed neutron kinetics are considered where several delayed neutron precursor groups may be born during each fission reaction.

These reactor kinetics equations can be formulated using a prompt neutron generation time or a mean neutron lifetime. Conceptually the neutron generation time is based on the production of neutrons, whereas the mean neutron lifetime is based on the destruction of neutrons. Neutron kinetics equations based on the neutron generation time are simpler mathematically than those based on mean neutron lifetime. Vigil [20] has demonstrated that the two forms are virtually equivalent and, therefore, the simpler equations based on neutron generation time are studied exclusively herein.

The dynamic equation which describes the rate of change of prompt neutrons is[21]

$$dn(t)/dt = \rho(t)n(t)/\ell \tag{3.1}$$

where

$n(t)$ = average neutron density (power, etc.)

ℓ = prompt neutron generation time, and

$\rho(t)$ = reactivity.

The analytic solution to equation (3.1) is

$$n(t) = n(0)\ \exp\left[\int_0^t \rho(\tau)\,d\tau/\ell\right] \tag{3.2}$$

where $n(0)$ = initial neutron density at $t = 0$. The independent variable t represents time for all of the neutron kinetics studies.

The dynamic equations which represent delayed neutron kinetics are

$$dn(t)/dt = [\rho(t) - \beta_{eff}]n(t)/\ell + \sum_{i=1}^{6} \lambda_i C_i(t) + S(t) \tag{3.3}$$

$$dC_i(t)/dt = \beta_i n(t)/\ell - \lambda_i C_i;\ i=1, \ldots, 6 \tag{3.4}$$

where the additional parameters and variables are

$C_i(t)$ = delayed neutron precursor density for group i,

$S(t)$ = extraneous neutron source,

λ_i = decay constant of group i of delayed neutron precursors,

β_i = the fraction of fission neutrons belonging to group i of delayed precursors,

β_{eff} = total effective fraction of fission neutrons which are delayed

$$= \sum_{i=1}^{6} \beta_i$$

The reactivity in both systems of equations is written in a general way as

$$\rho(t) = \rho_i(t) + \rho_f(t) \qquad (3.5)$$

where $\rho_i(t)$ represents the impressed reactivity input and $\rho_f(t)$ represents reactivity feedback effects.

Since $\rho(t)$ is generally nonlinear and/or time varying, analytic solutions to equations (3.3) and (3.4) seldom exist. Numerical methods (or analog computer solutions) are therefore required for their solution.

The values of λ_i and β_i for the six groups of delayed neutrons used in this work are those of uranium-235[13]. Table II shows their values. The values of neutron generation times range from $\ell = 10^{-8}$ second for fast burst reactors to $\ell = 10^{-3}$ second for slow thermal reactors. The values presented in Table II apply for fast fission of uranium-235. For comparison purposes, however, it is reasonable to use only one set of delayed neutron data for all values of ℓ.

TABLE II

Decay Constants and Delayed Neutron Fractions for Uranium-235; $\beta_{eff} = 0.0065$

Group Index i	Decay Constant λ_i	Relative Delay Fraction β_i/β_{eff}
1	0.0127	0.038
2	0.0317	0.213
3	0.115	0.188
4	0.311	0.407
5	1.40	0.128
6	3.87	0.026

Prompt Neutron Kinetics--Step Reactivity Input

The analytic solution for the case of prompt neutron kinetics with a step input of reactivity follows directly from equation (3.2):

$$n(t) = n(0) \exp [\rho_o t/\ell] \, . \tag{3.6}$$

In the above equation ρ_o represents the reactivity step with no feedback effects. Figure 1 is a plot of the solution--equation (3.6) for $\rho_o = 0.00064$, $\ell = 10^{-5}$ second, and $n(0) = 1.0$.

This very simple first order example serves to illustrate many of the advantages of using optimum integrating factors. The sequence of computation is carried through in detail. Initially ω and ζ are computed, then $n(\Delta t)$ is evaluated, and finally Δt for the next integration interval is obtained. To perform these calculations the method requires the first three derivatives of $n(t)$. These derivatives are generalized by

$$n^{(m)}(t) = \left(\frac{\rho_o}{\ell}\right)^m n(t) \tag{3.7}$$

Using the definitions of $\delta n^{(m)}$ we obtain

$$\delta n^{(m)} = \left(\frac{\rho_o}{\ell}\right)^m [n(\Delta t) - n(0)]. \tag{3.8}$$

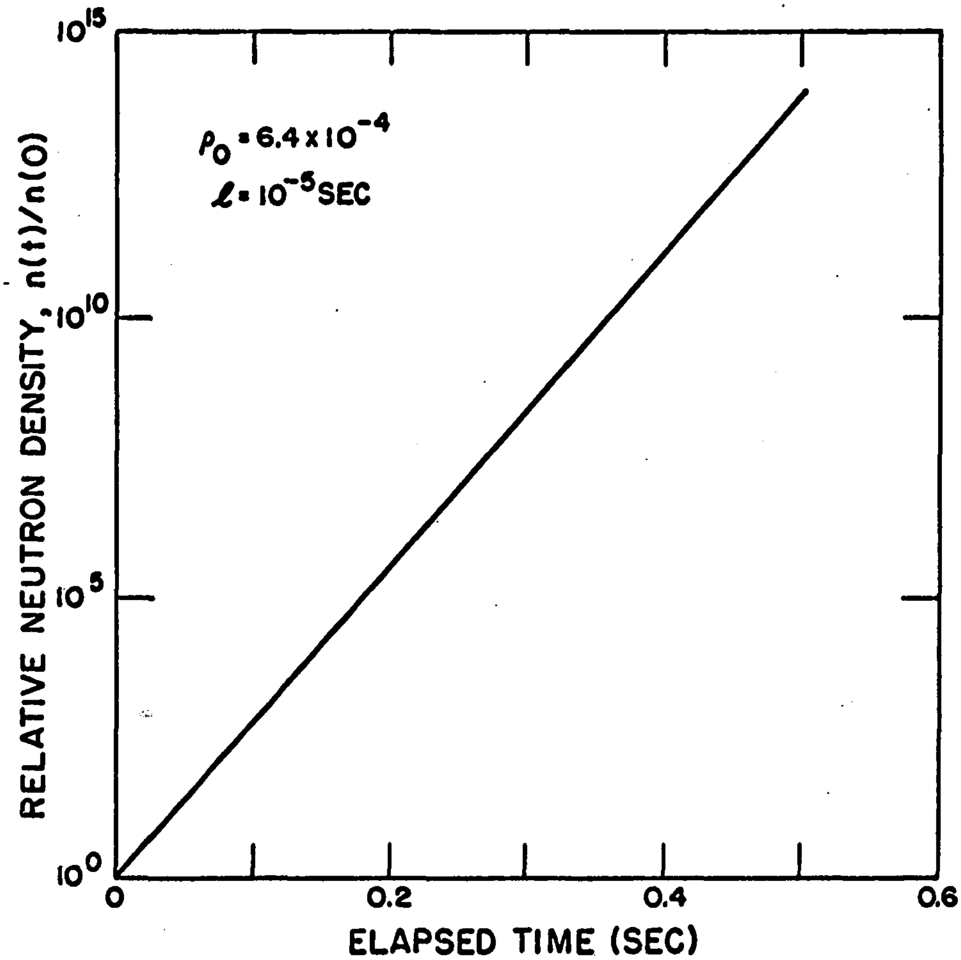

Fig. 1. Analytic Solution of Prompt Neutron Kinetics for a Step Reactivity

These relationships are sufficient to compute ω and ζ. The evaluation is

$$\omega_n^2 = \frac{\delta n^{(3)}\delta n^{(1)} - \delta n^{(2)}\delta n^{(2)}}{\delta n^{(2)}\delta n^{(0)} - \delta n^{(1)}\delta n^{(1)}} = \left(\frac{\rho_o}{\ell}\right)^2 \tag{3.9}$$

$$\zeta_n = -\left[\frac{\delta n^{(3)} + \omega_n^2 \delta n^{(1)}}{2\omega_n \delta n^{(2)}}\right] = -1 \tag{3.10}$$

where the subscript n refers to values associated with the dependent variable n(t). The corresponding values of the real and imaginary parts of the inverse time constants are

$$\alpha_n = \zeta_n \omega_n = -\frac{\rho_o}{\ell} \quad , \tag{3.11}$$

$$\beta_n = \sqrt{\omega_n^2 - \alpha_n^2} = 0 \tag{3.12}$$

Note that it has been determined that the appropriate exponent of the integrating factor is not complex, i.e., $\beta_n = 0$. The series approximation to $n(\Delta t)$ for this situation is

$$n(\Delta t) = n(0) + n^{(1)}(0)\Delta t + \frac{n^{(2)}(0)\Delta t^2}{2}$$

$$+ \frac{n^{(3)}(0)}{\alpha_n^3}\left[\frac{\alpha_n^2 \Delta t^2}{2} - \alpha_n \Delta t + 1 - \exp(-\alpha_n \Delta t)\right] . \tag{3.13}$$

Substituting equation (3.11) into equation (3.7) the derivatives of n(t) may be written

$$n^{(m)}(t) = (-\alpha_n)^m n(t) \ . \tag{3.14}$$

By evaluating the derivatives of n(t) at t = 0 using equation (3.14) and substituting these values into equation (3.13) the result is

$$\begin{aligned} n(\Delta t) &= n(0) \ \exp \ (-\alpha_n \Delta t) \\ &= n(0) \ \exp \ (\rho_o \Delta t/\ell) \ . \end{aligned} \tag{3.15}$$

Observe that the approximate series for $n(\Delta t)$ for a step input in reactivity has yielded the exact analytic solution. Further verification of this fact is obtained when the value of Δt is computed:

$$\Delta t = \left\{ \frac{24\epsilon \left| n(\overline{\Delta t}) \right| \left[\bar{1} + \frac{\alpha_n \Delta t}{5} \right]}{\left| \delta n^{(3)} + \alpha_n \delta n^{(2)} \right|} \right\}^{\frac{1}{3}} \ . \tag{3.16}$$

The denominator within the brackets, using previously derived relationships, is identically zero. This implies that an infinite value for Δt is sufficient to guarantee the required relative truncation error, ϵ. Figure 2 is a plot of the accumulated error as a function of time using optimum integrating factors. For the graph illustrated, $\epsilon = 10^{-6}$. The

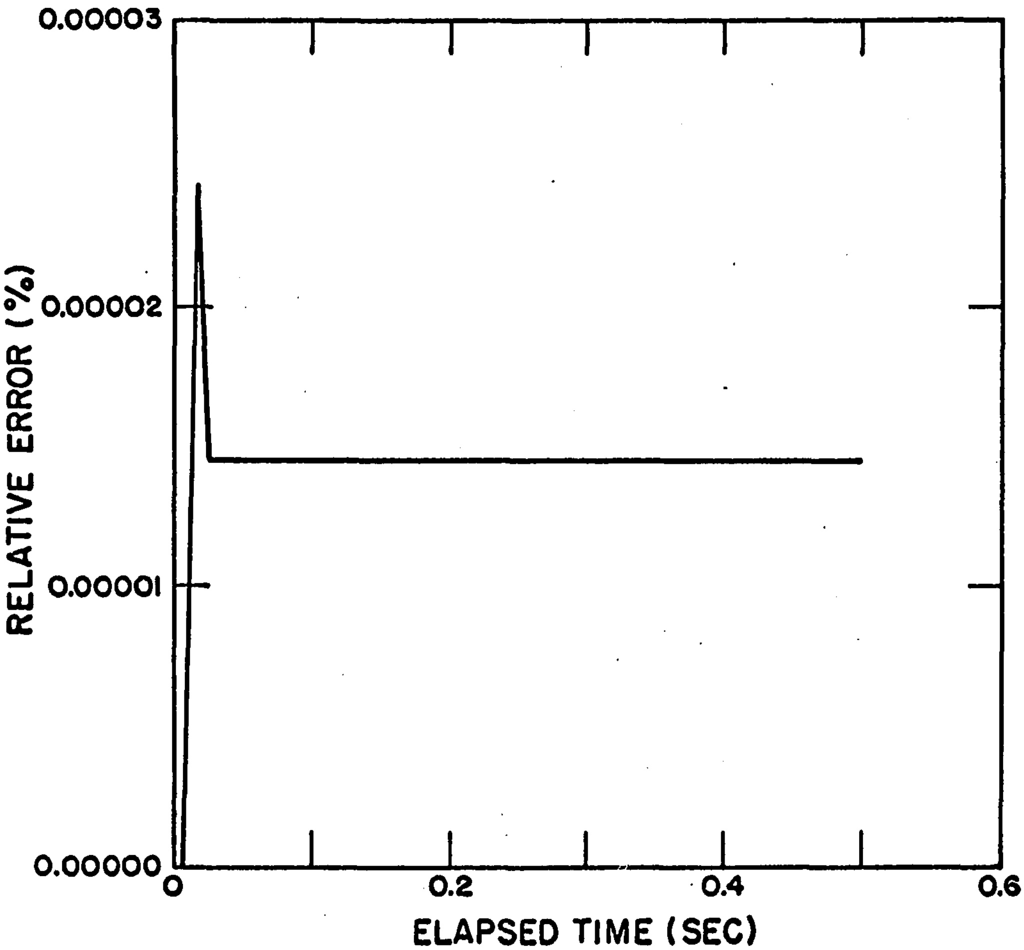

Fig. 2. Accumulated Error Using Optimum Integrating Factors for a Step Reactivity

initial error results from the fact that a Taylor series was used to initiate the solution. The parameter α_n was not computed until the first integration interval was traversed. Figure 3 is a plot of the computed value of α_n as a function of time.

In contrast to optimum integrating factors, it can be demonstrated that the integration Δt computed using continuous analytic continuation is limited severly by the values of ϵ and neutron generation time ℓ. For this situation Δt is computed from the equation

$$\Delta t = \left[\frac{24\epsilon\,|n(\Delta t)|}{|\delta n^{(3)}|}\right]^{\frac{1}{3}}$$

or

$$\left(\frac{\rho_o \Delta t}{\ell}\right) = \left[\frac{24\epsilon\,|n(\Delta t)|}{|n(\Delta t) - n(0)|}\right]^{\frac{1}{3}} \tag{3.17}$$

The relationship between $n(\Delta t)$ and $n(0)$ is

$$n(\Delta t)(1 + \epsilon) \le n(0) \exp\,(\rho_o \Delta t/\ell)\ . \tag{3.18}$$

The following nonlinear equation for $\rho_o \Delta t/\ell$ results:

$$\left(\frac{\rho_o \Delta t}{\ell}\right) = \left[\frac{24\epsilon}{1 - (1 + \epsilon)/\exp\,(\rho_o \Delta t/\ell)}\right]^{\frac{1}{3}} \tag{3.19}$$

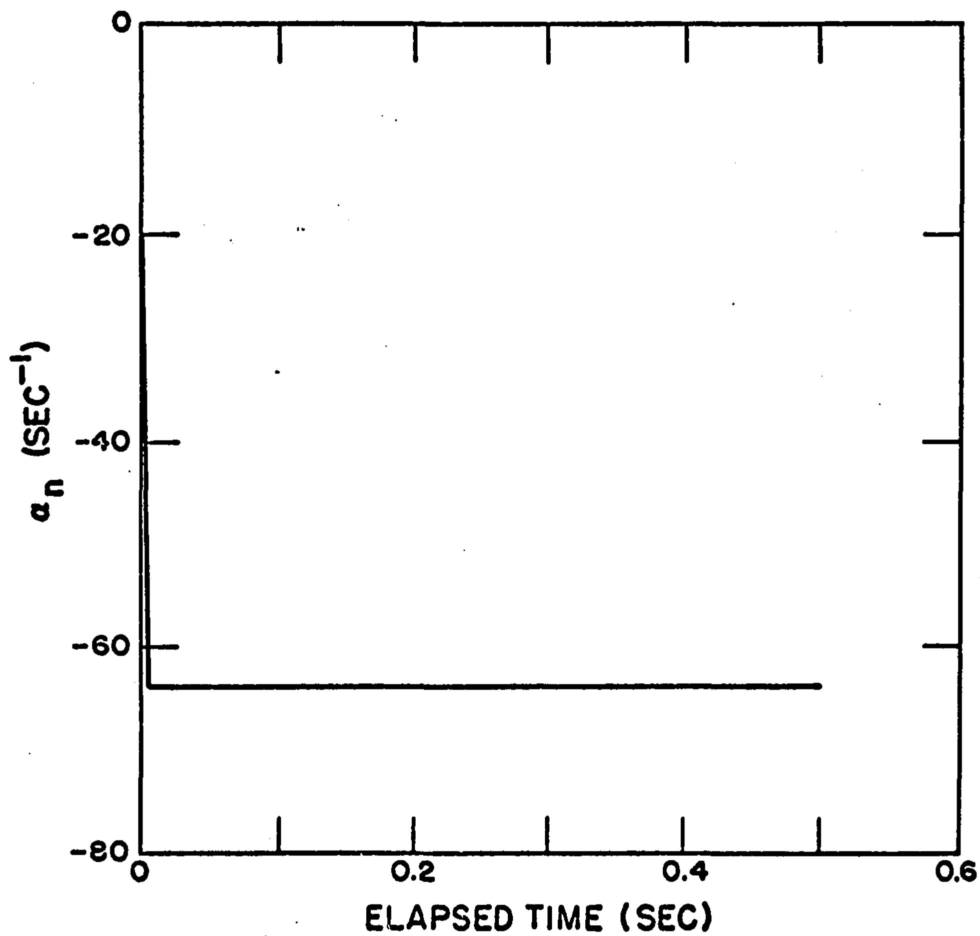

Fig. 3. Computed Inverse Time Constant for Neutron Density

Figure 4 is a plot of the accumulated relative error in the solution using continuous analytic continuation for $\epsilon = 10^{-6}$. Clearly the accumulated error increases linearly with time, whereas (as illustrated in Figure 2) the accumulated error using optimum integrating factors is a constant value of 1.45×10^{-6}. Figure 5 is a plot of $\rho_0 \Delta t/\ell$ as a function of ϵ as determined from equation (3.19). The value of Δt determined from Figure 5 using ρ_0, ℓ, and ϵ for this problem is

$$\Delta t = 1.125 \times 10^{-3} \text{ second.}$$

The average value determined from the computer solution using continuous analytic continuation was

$$\Delta t_{actual} = 1.05 \times 10^{-3} \text{ second.}$$

This example vividly illustrates some of the advantages of using optimum integrating factors. The criterion for computing α_n has given rise to an integration step Δt which is obviously the maximum--infinite in this case regardless of the magnitude of ℓ. Whenever the solution deviates from pure exponential behavior, however, the magnitude of Δt will be finite.

Prompt Neutron Kinetics--Ramp Reactivity Input

Another first order prompt neutron kinetics problem is that of a ramp input in reactivity with no feedback effects.

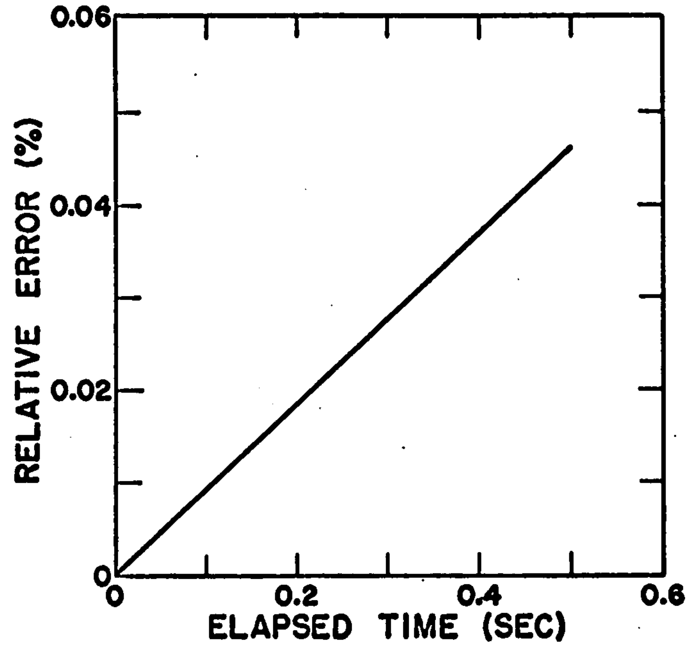

Fig. 4. Accumulated Error Using Continuous Analytic Continuation for a Step Reactivity

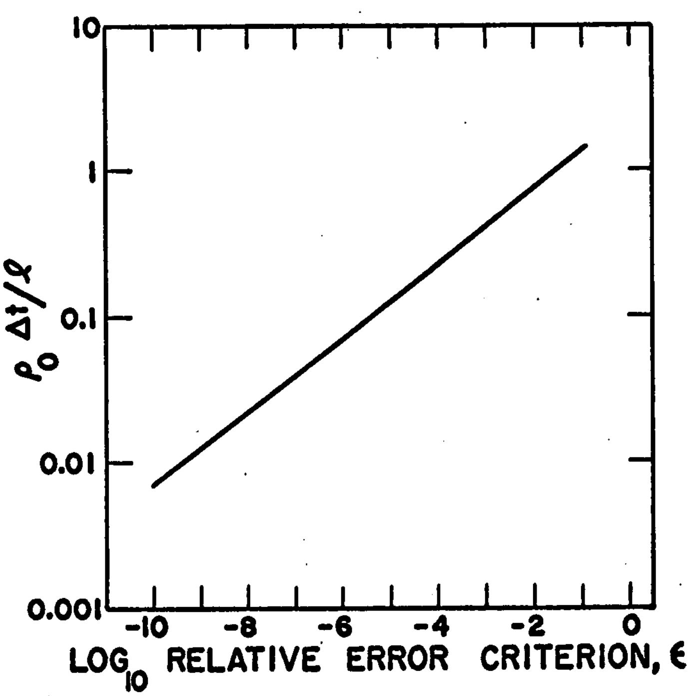

Fig. 5. Solution of Equation (3.19) for $\rho_0\Delta t/\ell$

In this situation the approximate formula for n(t) is not exact but the behavior is near exponential. For this reason a significant increase in the average Δt is achieved using optimum integrating factors. The reactivity has the form

$$\rho(t) = at \; . \tag{3.20}$$

The analytic solution for this problem is

$$n(t) = n(0) \exp\left[\frac{at^2}{2\ell}\right] \tag{3.21}$$

Figure 6 is a plot of n(t) for the case where $n(0) = 1$, $a = 2.1 \times 10^{-3}$ sec^{-1}, and $\ell = 8 \times 10^{-9}$ second. Figure 7 shows the ramp reactivity as given in equation (3.20) as a function of time.

The average integration step size for $\epsilon = 10^{-6}$ using optimum integrating factors was $\Delta t = 1.57 \times 10^{-4}$ second--using continuous analytic continuation, $\Delta t = 4.1 \times 10^{-5}$ second. This represents better than a three-fold decrease in computer running time. A comparison of solution accuracy using the two methods is shown in Figure 8. Although the error criterion was the same for both solutions, the maximum accumulated error using optimum integrating factors was approximately one fifth as large--maximum error = 0.0071 %. This indicates that equation (2.21) used to compute Δt is conservative. The same accuracy achieved with continuous analytic continuation could be obtained by increasing ϵ and thereby decreasing the total

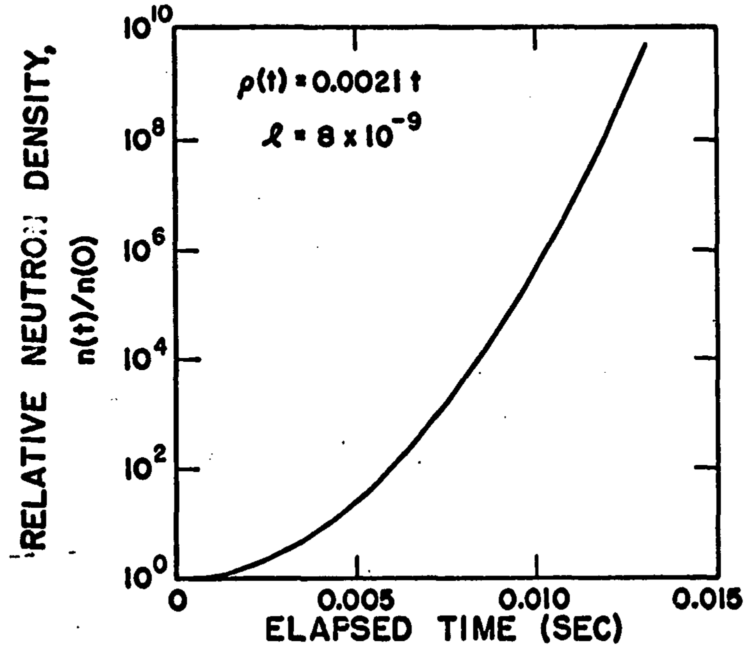

Fig. 6. Analytic Solution for the Neutron Density for a Ramp Reactivity

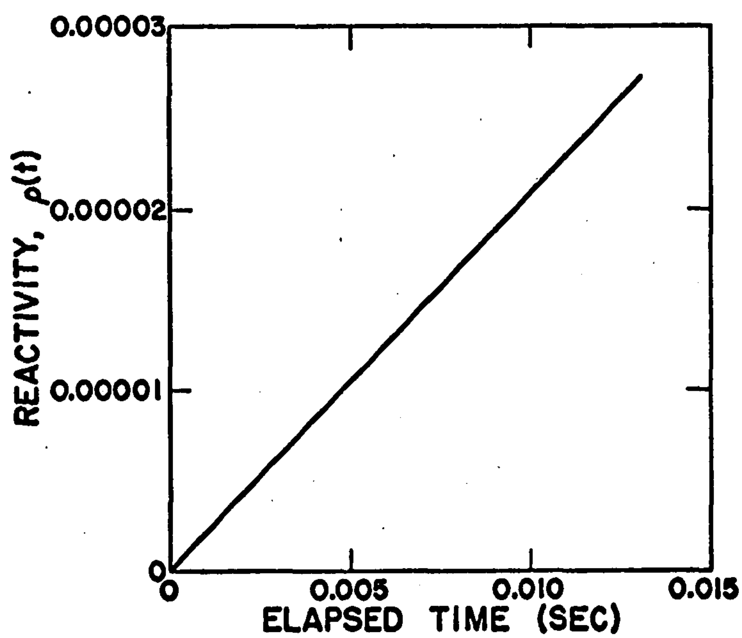

Fig. 7. Ramp Reactivity for Prompt Neutron Kinetics

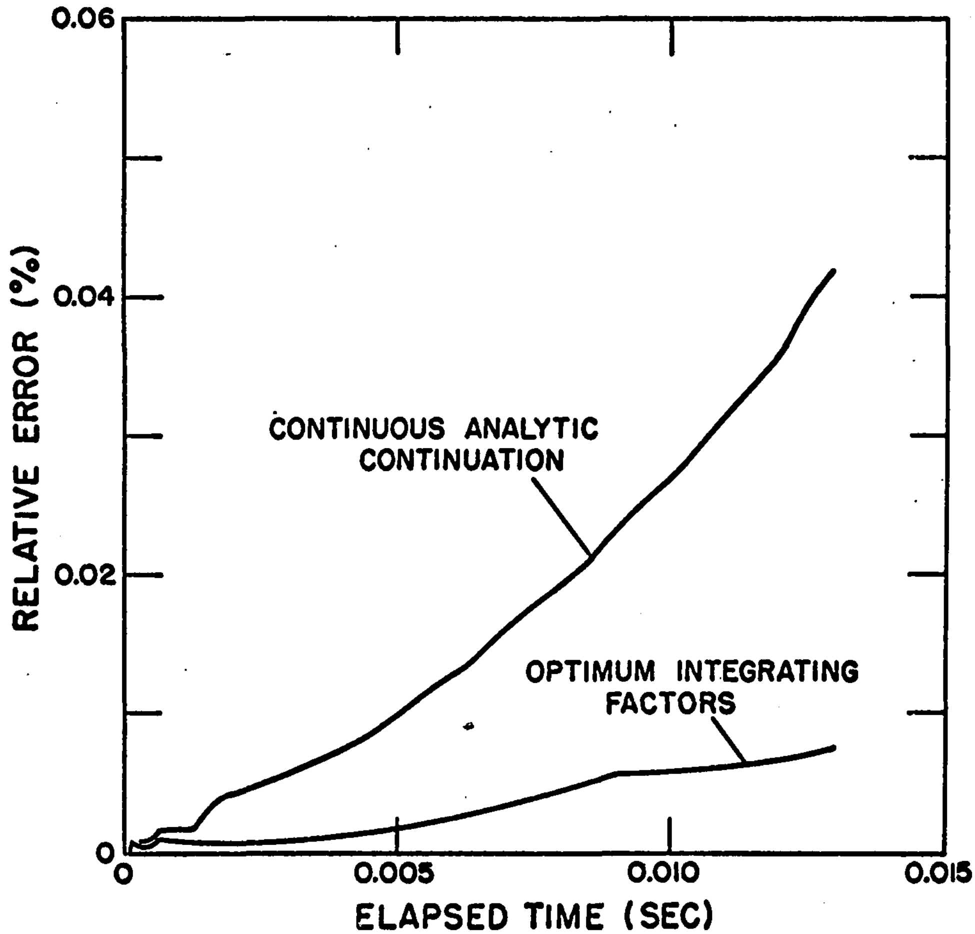

Fig. 8. Comparison of the Accumulated Error Using Analytic Continuation and Optimum Integrating Factors

solution computational time. This was observed with respect to all of the problems studied where analytic solutions exist.

Figure 9 illustrates the computed value of α_n for this case. The approximate relationship for this parameter is

$$\alpha_n(t) = - n^{(3)}(t)/n^{(2)}(t)$$

$$= - \frac{\rho(t)}{\ell}\left[\frac{3\ell + \rho(t)t}{\ell + \rho(t)t}\right] \tag{3.22}$$

The computed curve does not differ from this relationship by more than 5% at any point. The asymptotic value of $\alpha_n(t)$, where $t \to \infty$, is

$$\lim_{t \to \infty} \alpha_n(t) = - \rho(t)/\ell \tag{3.23}$$

This asymptotic value, as noted on Figure 9, is being approached.

Prompt Neutron Kinetics--Sinusoidal Variation in Reactivity

The first order examples are concluded with the problem of prompt neutron kinetics with a sinusoidal variation in reactivity and no feedback effects. The reactivity has the form

$$\rho(t) = \rho_o \sin \omega t. \tag{3.24}$$

The analytic equation for n(t) is

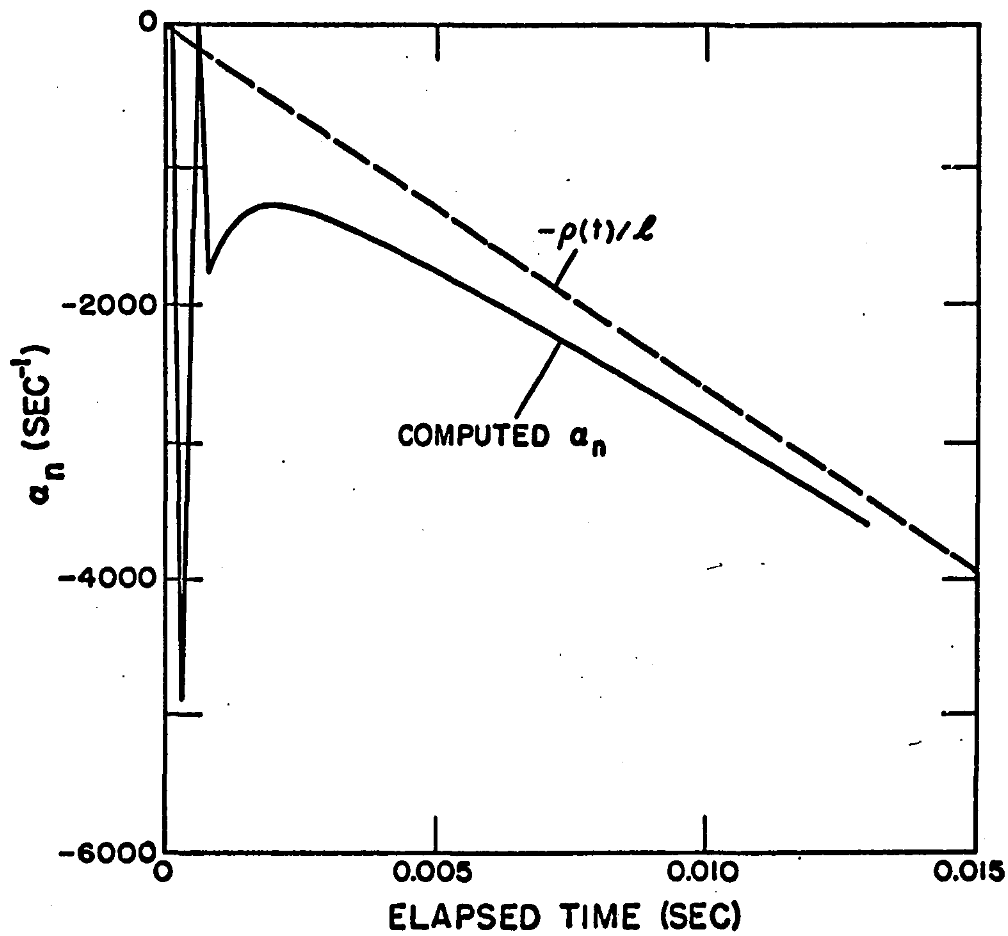

Fig. 9. Computed Inverse Time Constant for Neutron Density for a Ramp Reactivity

$$n(t) = n(0)\ \exp\left[\frac{\rho_o}{\ell\omega}(1 - \cos\omega t)\right]. \qquad (3.25)$$

Figure 10 shows the sinusoidal reactivity function for $\rho_o = 5 \times 10^{-4}$ and $\omega = 10$ second^{-1}. The solution n(t), as given in equation (3.25) for this reactivity function, is illustrated in Figure 11. For this case n(0) = 1 and $\ell = 10^{-5}$ second.

The solution for this case does not exhibit near exponential behavior throughout the integration interval. Two cycles of sinusoidal variation are plotted which substantiate this fact. Results using optimum integrating factors, however, are not hampered by this condition. In the vicinities where n(t) achieves its maximum values, the method of optimum integrating factors predicts a complex exponent for the integrating factor. Figures 12 and 13 are plots of the computed values of $\alpha_n(t)$ and $\beta_n(t)$ obtained.

The average time step obtained using optimum integrating factors was $\Delta t = 4.3 \times 10^{-2}$ second; using continuous analytic continuation, $\Delta t = 1.9 \times 10^{-3}$ second. A comparison of the accumulated error for $\epsilon = 10^{-6}$ using both methods can be seen on Figures 14 and 15. The maximum accumulated error using optimum integrating factors is seen to be -0.002%; for the other method the maximum error was 0.045%. The accumulated error of Figure 14 oscillated in behavior increasing its maximum only slightly with each cycle of the solution.

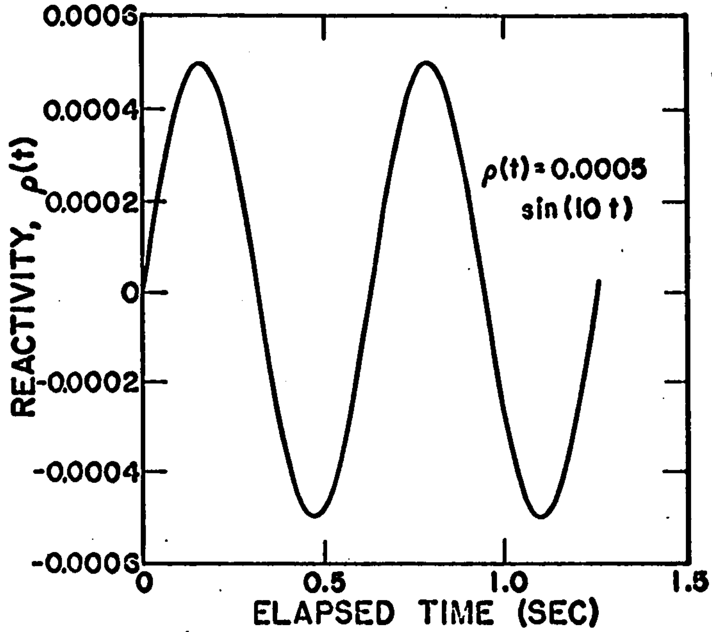

Fig. 10. Sinusoidal Reactivity for Prompt Neutron Kinetics

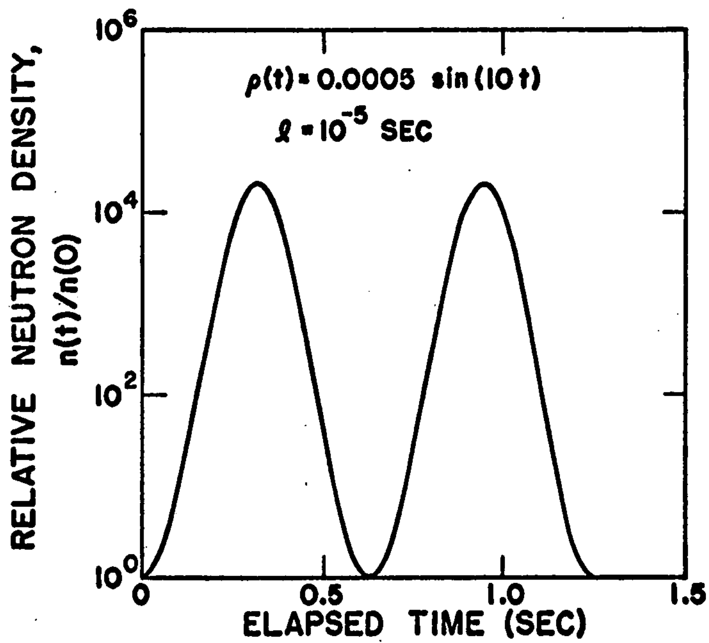

Fig. 11. Analytic Solution of the Neutron Density for a Sinusoidal Variation in Reactivity

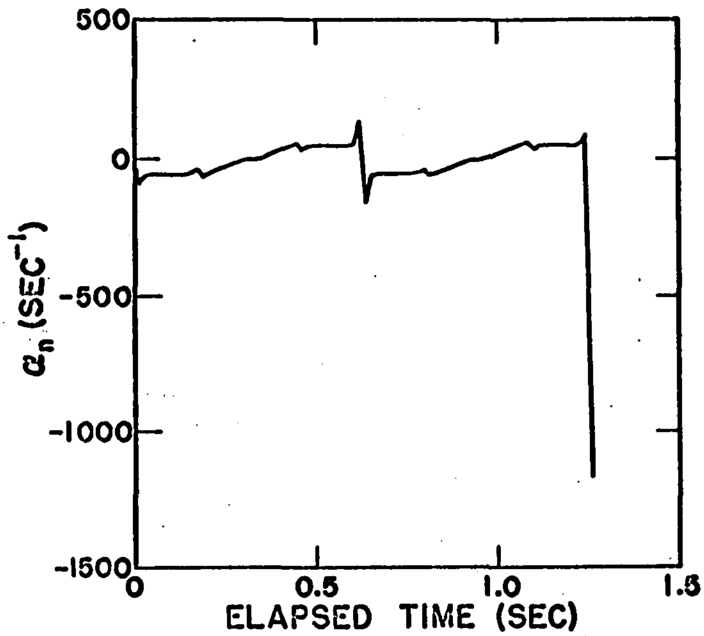

Fig. 12. Computed α_n for Prompt Neutron Kinetics with Sinusoidal Reactivity

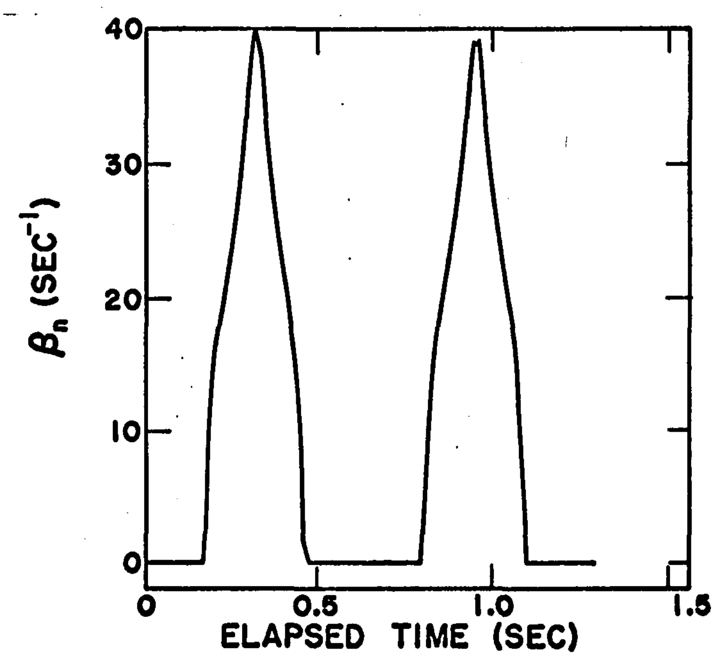

Fig. 13. Computed β_n for Prompt Neutron Kinetics with Sinusoidal Reactivity

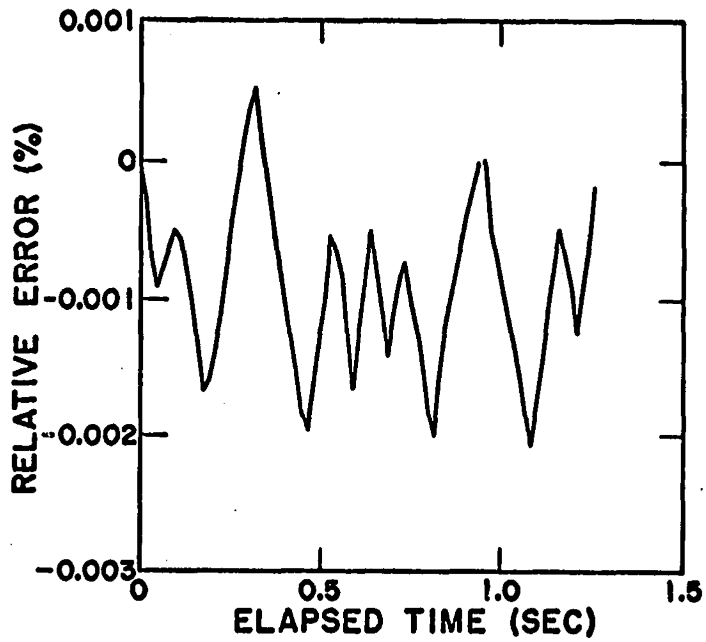

Fig. 14. Accumulated Error in Neutron Density Using Optimum Integrating Factors for Sinusoidal Reactivity

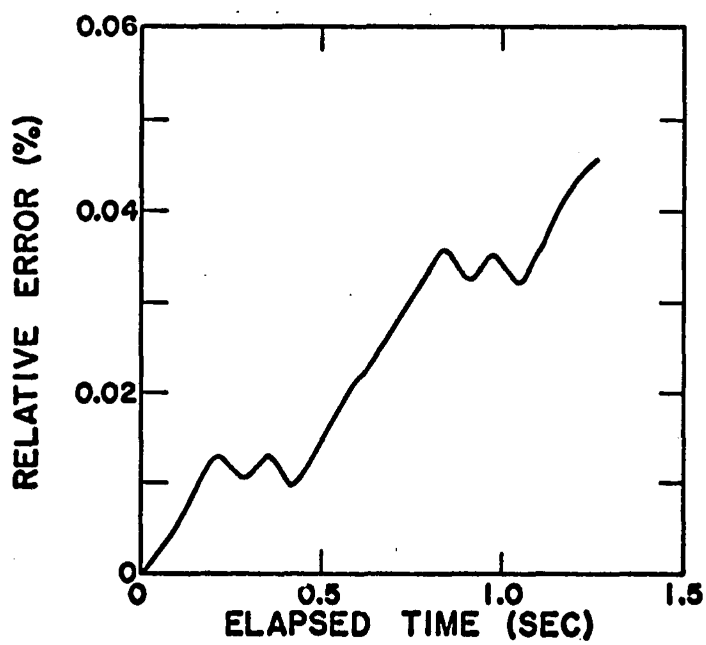

Fig. 15. Accumulated Error in Neutron Density Using Analytic Continuation for Sinusoidal Reactivity

In contrast, however, continuous analytic continuation produced an accumulated error having an almost monotonically increasing behavior.

In this example again a larger value for the error criterion ϵ could have been utilized, decreasing computational time without significantly increasing the accumulated error. Hence, the equation for determining Δt, knowing both α_n and β_n, is conservative for this problem.

The remainder of the studies presented are higher-than-first order examples. No analytic solutions are known to exist for these cases. They further demonstrate that computational times are reduced using optimum integrating factors. They also illustrate the ease of extending the method to solutions of high order problems.

Delayed Neutron Kinetics--Sinusoidal Variation in Reactivity

The method of optimum integrating factors was tested on a second order problem of delayed neutron kinetics. The problem represents a half-period of sinusoidal reactivity input ($\rho_o < \beta_{eff}$) using one averaged group of delayed neutrons. The solution has some characteristics of a sub-prompt-critical self limiting power excursion. Szeligowski and Hetrick [18] have compared a number of the integral equation numerical methods in solving this test problem. Their results indicate that the collocation method of Brittan [3] and Adler and Cohen's method yield superior accuracy and larger integration step sizes for a large range of neutron generation time. The other methods compared were Hansen's method [9] and the Laplace transform [12] method. A direct comparison of optimum integrating factors is obtained with those methods by determining the average Δt required for the solution.

The reactor kinetics model used here is

$$dn(t)/dt = [\rho(t) - \beta_{eff}]\, n(t)/\ell + \lambda C(t) \tag{3.26}$$

$$dC(t)/dt = \beta_{eff} n(t)/\ell - \lambda C(t) \tag{3.27}$$

$$\rho(t) = \rho_o \sin(\pi t/T) \;. \tag{3.28}$$

In these equations C(t) represents an average delayed neutron precursor density and λ is the average decay constant; T is the half-period of the sinusoidal reactivity. The sinewave amplitude ρ_o is arbitrarily related to the period using the approximate reactor inhour equation by

$$\rho_o = \frac{8\beta_{eff}}{8 + \lambda T} \;. \tag{3.29}$$

The values used in this study were $\beta_{eff} = 0.0079$, $\lambda = 0.077\ \mathrm{sec}^{-1}$, $n(0) = 1$, and $\ell = 10^{-7}$ second. For small values of ℓ (roughly $\ell \le 10^{-5}$ sec) a good approximation to n(t) may be obtained using the prompt-jump approximation [2] which is

$$n(t) = \frac{\beta_{eff} n(0)}{\beta_{eff} - \rho(t)} \exp\left[-\lambda t + \frac{\beta_{eff}\lambda T}{\pi\sqrt{\beta_{eff}^2 - \rho_o^2}} \left(\sin^{-1}\frac{\rho_o}{\beta_{eff}} - \sin^{-1}\frac{\rho_o^2 - \beta_{eff}\rho(t)}{\rho_o\beta_{eff} - \rho_o\rho(t)} \right) \right] \tag{3.30}$$

Figure 16 is a plot of $\rho(t)$ for T = 350 seconds. The solution to n(t) obtained using optimum integrating factors with the relative error criterion $\epsilon = 10^{-4}$ is shown in Figure 17. For this case $\rho_o = 1.808 \times 10^{-3}$.

The average Δt required to generate the solution using optimum integrating factors was $\Delta t = 0.97$ second. Szeligowski and Hetrick report that for T = 350 seconds only the collocation technique yields comparable accuracy for $\Delta t > 1$ second. Optimum integrating factors would appear to be superior to all of the other methods on this basis. An error comparison of the computed n(t) with equation (3.30) is shown in Figure 18. At one point the maximum error is -0.52%; the mean error appears to be zero.

The computational time using optimum integrating factors was 2.58 seconds on a CDC 6600 computer; using continuous analytic continuation the problem solution was not completed in the required 1.0 minute time limit on the same computer. This same problem was run using $\ell = 10^{-3}$, 10^{-4},

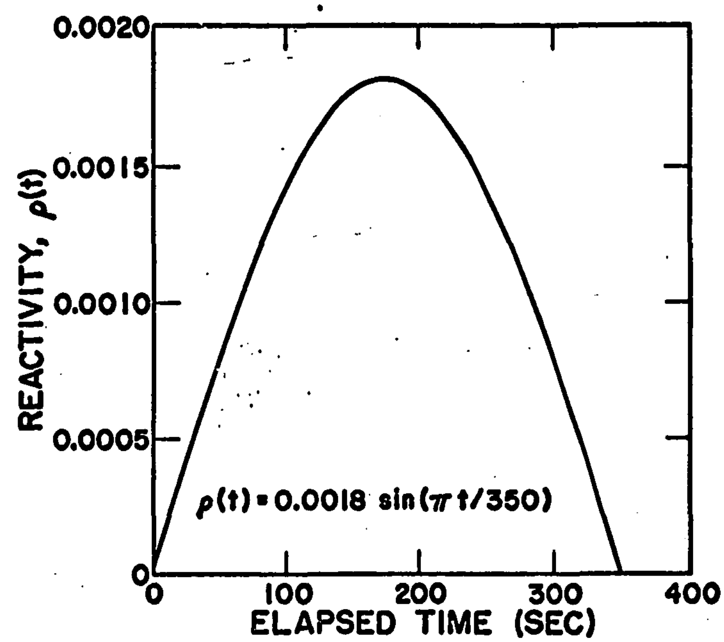

Fig. 16. Sinusoidal Reactivity for Delayed Neutron Kinetics

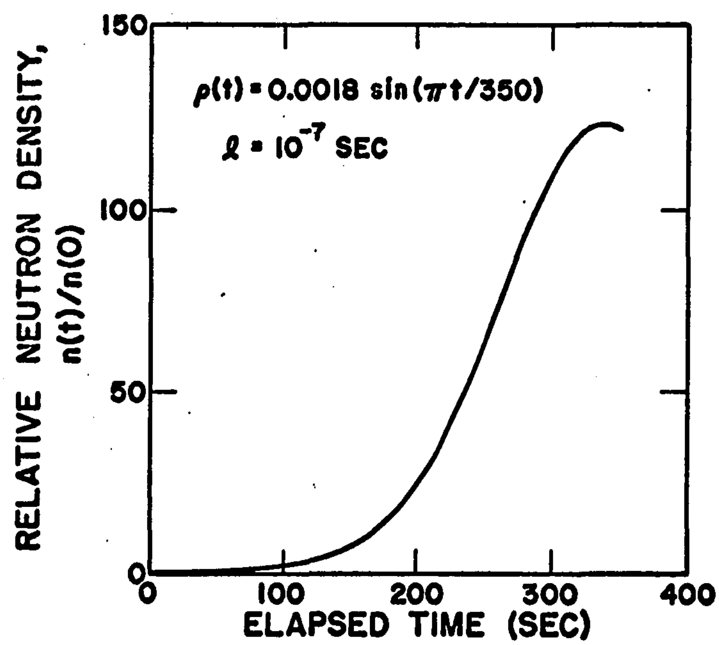

Fig. 17. Numerical Solution for the Neutron Density Using Optimum Integrating Factors

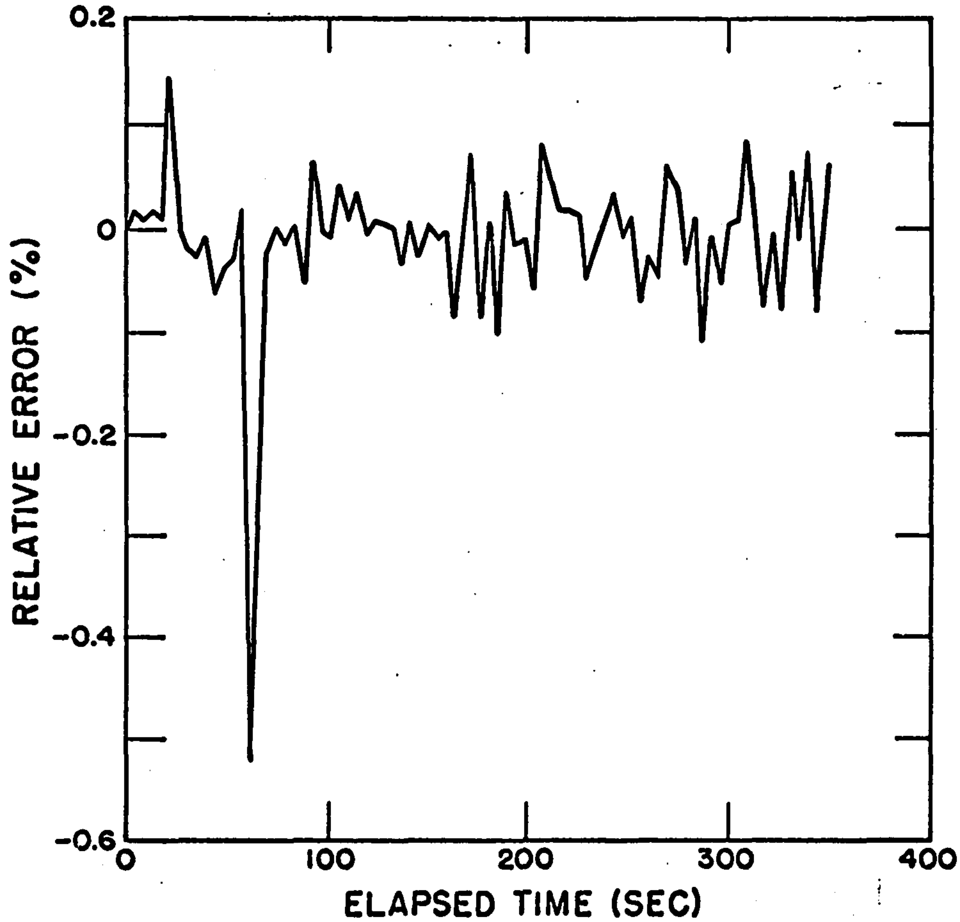

Fig. 18. Relative Error of the Numerical Solution for Neutron Density Compared to the Prompt Jump Approximation

10^{-5}, ..., 10^{-8} second. The solution, which is not a sensitive function of ℓ --note that equation (3.30) is independent of ℓ --using optimum integrating factors required running times ranging from 1.61 seconds to 2.64 seconds. In contrast finite difference methods and continuous analytic continuation are quite sensitive to the parameter ℓ ; decreasing ℓ increases computational time for this problem. Continuous analytic continuation is by no means, however, as slow a technique as finite difference methods are.

Figure 19 is a plot of $\alpha_n(t)$ computed for this problem. The computed curve is everywhere, with the exception of t = 0, within a small fraction of one percent equal to

$$\alpha_n(t) = \frac{\beta_{eff} - \rho_o \sin(\pi t/T)}{\ell} \tag{3.31}$$

As ℓ was increased it was observed that $\alpha_n(t)$ deviated farther and farther from equation (3.31). This results because as ℓ increases the coupling between n(t) and C(t) changes. The presence of delayed neutrons, in other words, influences the shape of n(t) for large ℓ .

<u>Delayed Neutron Kinetics--Compensated Ramp Reactivity</u>

One neutron kinetics problem that appears throughout the literature on numerical solutions of dynamic nuclear reactor systems is that of a ramp input in reactivity with feedback proportional to the total energy released[9,12,20]. The reactor kinetics model is the six delayed neutron group model

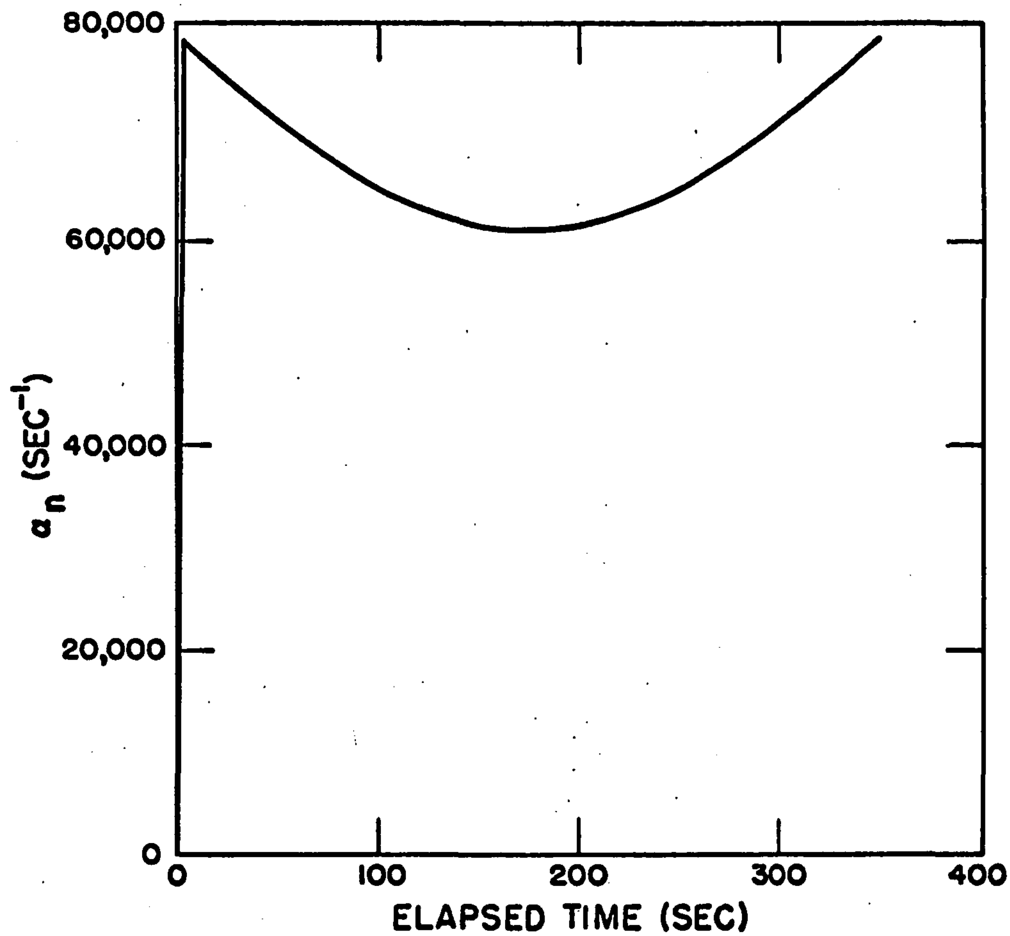

Fig. 19. Computed α_n for Delayed Neutron Kinetics with Sinusoidal Reactivity

represented by equations (3.3) and (3.4). The reactivity relationship in this situation is

$$\rho(t) = at - bE(t) \tag{3.32}$$

where E(t) represents the total energy release. It is determined by the differential equation

$$dE(t)/dt = n(t) - n(0) , \tag{3.33}$$

Including equation (3.33) the order of this system of differential equations is 8.

The delayed neutron data is that presented in Table II. The additional parameters used were $a = 0.064\ \text{sec}^{-1}$, $b = 3.76 \times 10^{-5}\ \text{sec}^{-1}$, $\ell = 10^{-5}$ second, $E(0) = 0$, and $n(0) = 1$. The initial conditions for the delayed neutron precursor groups were determined from the steady state relationship

$$C_i(0) = \beta_i n(0)/\lambda_i \ell \ ; \ i=1, \ldots, 6 \ . \tag{3.34}$$

The relative error criterion used was $\epsilon = 10^{-4}$.

The computed solution for n(t) using optimum integrating factors is presented in Figure 20. Figures 21 and 22 show the solutions for the reactivity and energy release. Although no analytic solution for n(t) exists, the results are in excellent agreement with predicted behavior. In the case of a compensated ramp reactivity as t approaches infinity the total reactivity will approach zero. Combining equations (3.32) and (3.33) the asymptotic value of n(t) can be predicted.

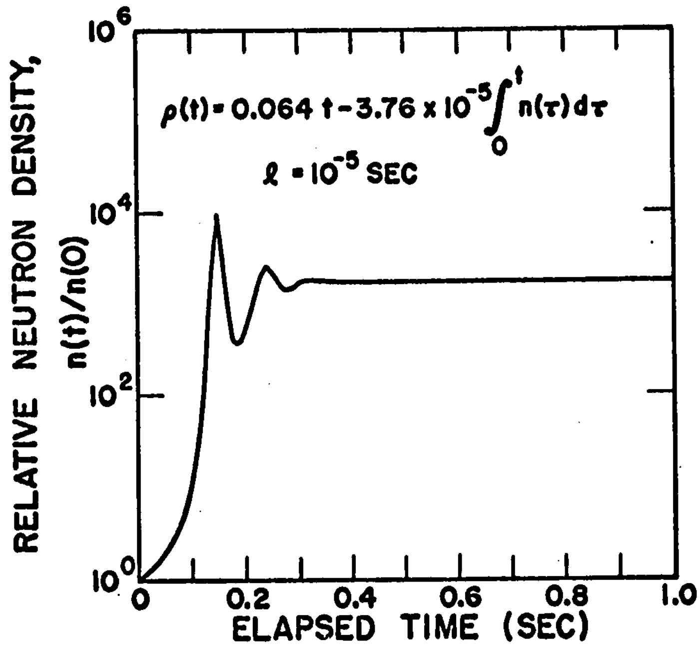

Fig. 20. Numerical Solution for the Neutron Density with a Compensated Ramp Reactivity

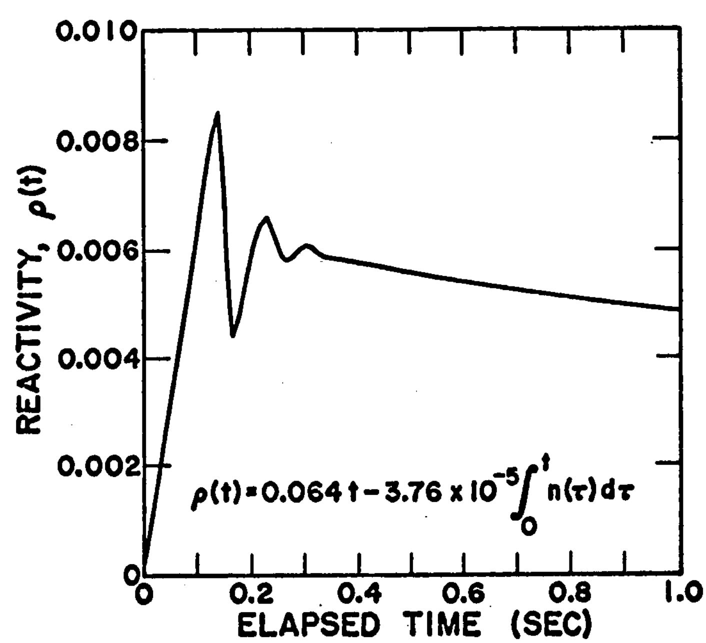

Fig. 21. Compensated Ramp Reactivity for Delayed Neutron Kinetics

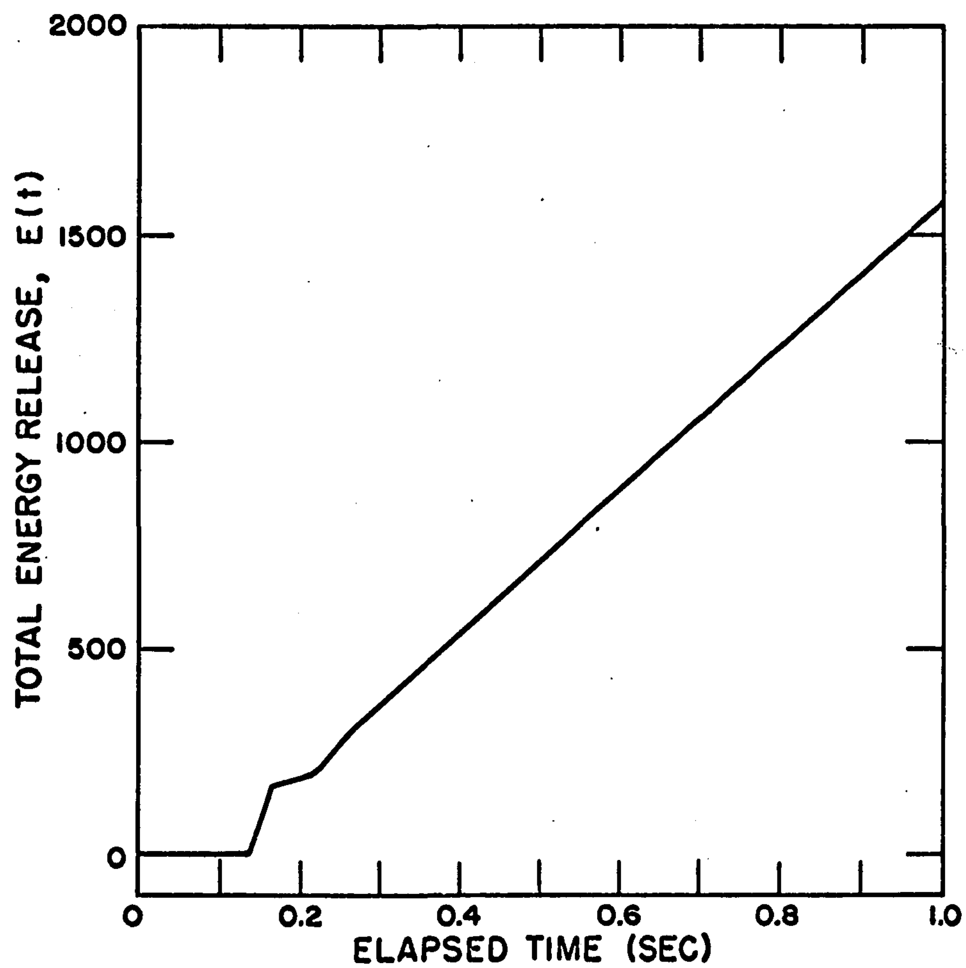

Fig. 22. Total Energy Release for Delayed Neutron Kinetics with Compensated Ramp Reactivity

$$\lim_{t \to \infty} \rho(t) = 0 = at - b\int_0^t [n(\tau) - n(0)]d\tau \qquad (3.35)$$

Differentiating the right hand side of equation (3.35) with respect to time the result is

$$\lim_{t \to \infty} n(t) = n(0) + a/b = 1703.2 \qquad (3.36)$$

Figure 20 verifies that n(t) has indeed achieved its asymptotic value to within one percent after 1 second. Further, $\rho(t)$ (Figure 21) is approaching zero and E(t) (Figure 22) has nearly achieved its asymptotic relationship,

$$\lim_{t \to \infty} E(t) = at/b = 1702.2t \quad .$$

A comparison of computer running times for this method with continuous analytic continuation was made. The results were 1.15 seconds for optimum integrating factors and 15.2 seconds for the other method. Vigil demonstrated that continuous analytic continuation is faster by a factor of 25 over the Laplace transform method used in the RTS code for the same problem.

Oscillating Feedback in a Nuclear Reactor

A nonlinear kinetics problem was investigated in which the reactivity feedback transfer function exhibits complex poles corresponding to a damped oscillation. It was felt that such a system would be a good test for the method of optimum integrating factors. The reactor model, a boiling water homogeneous reactor[6], was used by Torlin[19] in a study of autonomous nonlinear oscillations.

If θ is the time constant of the liquid phase, ignoring mechanical inertia, and φ is the time constant of the steam phase the reactivity to power transfer function for periodic behavior is

$$\frac{n(0)\delta R(s)}{\delta N(s)} = \frac{k}{1 + \varphi s + \theta\varphi s^2} \tag{3.37}$$

where $s = i\omega$, ω is the frequency of oscillation, k is the gain and n(0) is the initial neutron density. Equation (3.37) corresponds to a second order differential equation relating the feedback reactivity whose linearized Laplace transform is $\delta R(s)$, to the neutron density, whose Laplace transform is $\delta N(s)$.

The equivalent time domain equations are represented as

$$\rho(t) = \rho_o - [\rho_1(t) - \rho_1(0)] \ , \tag{3.38}$$

$$d\rho_1(t)/dt = [\rho_2(t) - \rho_2(0)]/\varphi \ , \tag{3.39}$$

$$d\rho_2(t)/dt = \Big\{k[n(t) - n(0)]/n(0) - \rho_2(t) - \rho_1(t) + \rho_2(0) + \rho_1(0)\Big\}/\theta \ , \tag{3.40}$$

where ρ_o is the input reactivity--a constant for this study. Here $\rho_1(t)$ represents the feedback reactivity. These equations, combined with the six group delayed neutron kinetics model of equations (3.3) and (3.4), form a ninth order system.

Results using optimum integrating factors are presented in Figures 23 through 31. The parameters used for the solution were:

$$\epsilon = 10^{-4} \qquad n(0) = 1.0$$
$$\rho_o = 0.3\ \beta_{eff} \qquad \ell = 10^{-4} \text{ second}$$
$$\rho_1(0) = 0.001 \qquad \varphi = 1.0 \text{ second}$$
$$\rho_2(0) = 0.001 \qquad \theta = 1.0 \text{ second}$$
$$k = 0.2\ \beta_{eff} \qquad C_i(0) = \beta_i n(0)/\lambda_i \ell$$

For the values of θ and φ stated, the feedback period of oscillation is 2π seconds. Figure 24 shows that the period of oscillation for this ninth order system is approximately 5.3 seconds. The solution is carried for three cycles of reactivity oscillation. The values of the steam and liquid time constants used in this study are related such that the feedback reactivity $\rho_1(t)$ is damped at a substantial rate.

Figure 23 shows the neutron density. The relatively high damping rate is observed after the first cycle of the solution where the neutron density increases monotonically. Total reactivity is shown in Figure 24. The neutron density,

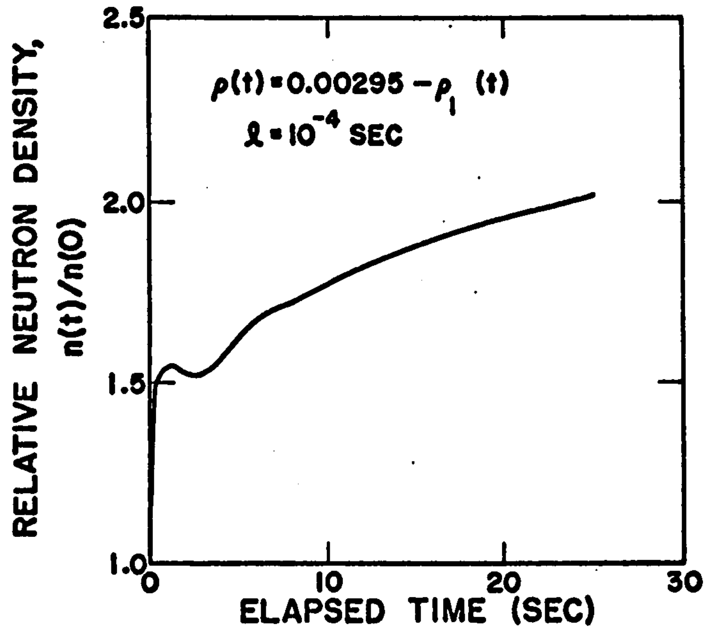

Fig. 23. Numerical Solution for the Neutron Density in an Oscillating Feedback Reactor

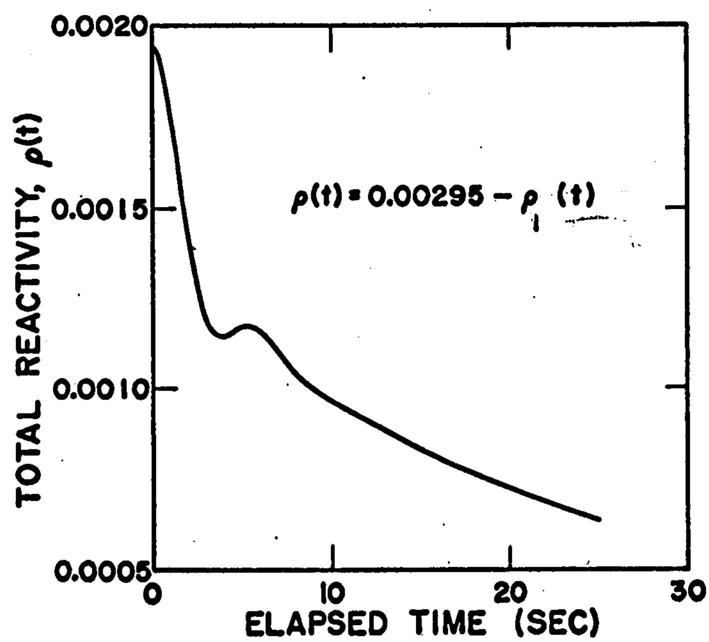

Fig. 24. Total Reactivity in an Oscillating Feedback Reactor

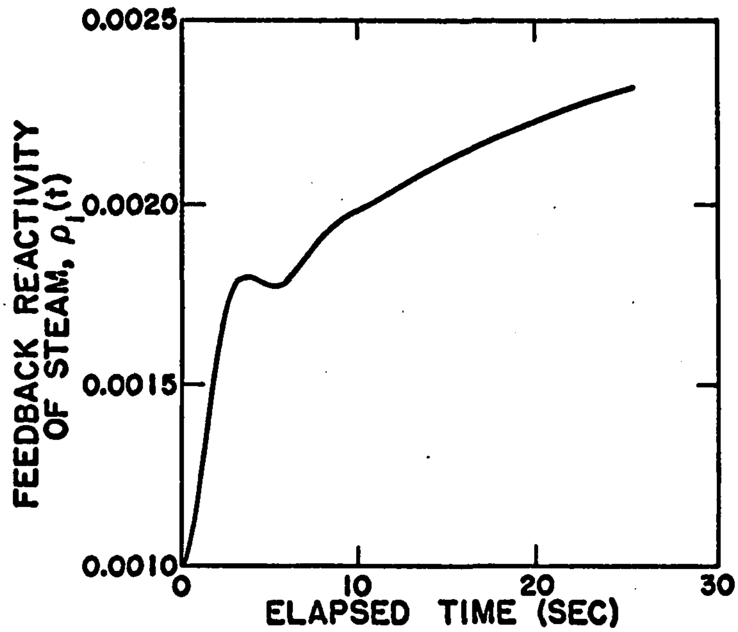

Fig. 25. Feedback Reactivity of Steam Phase in an Oscillating Feedback Reactor

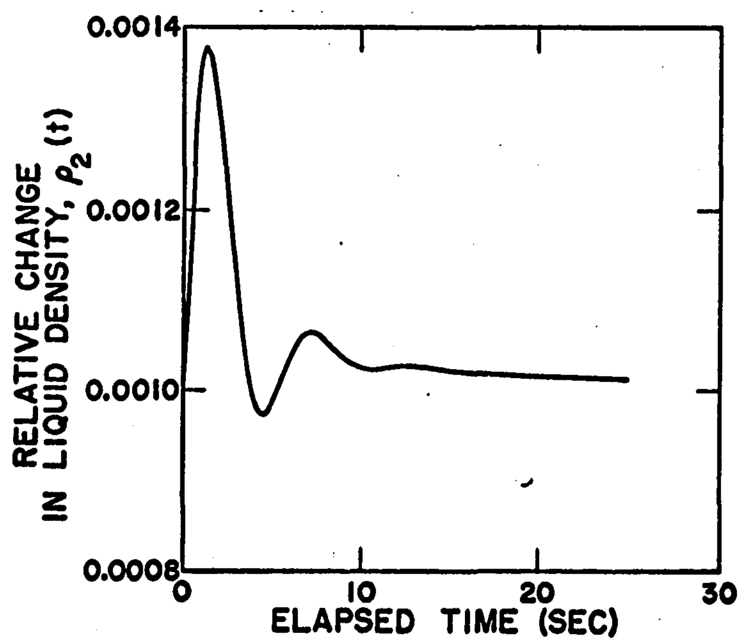

Fig. 26. Relative Change of the Liquid Density in an Oscillating Feedback Reactor

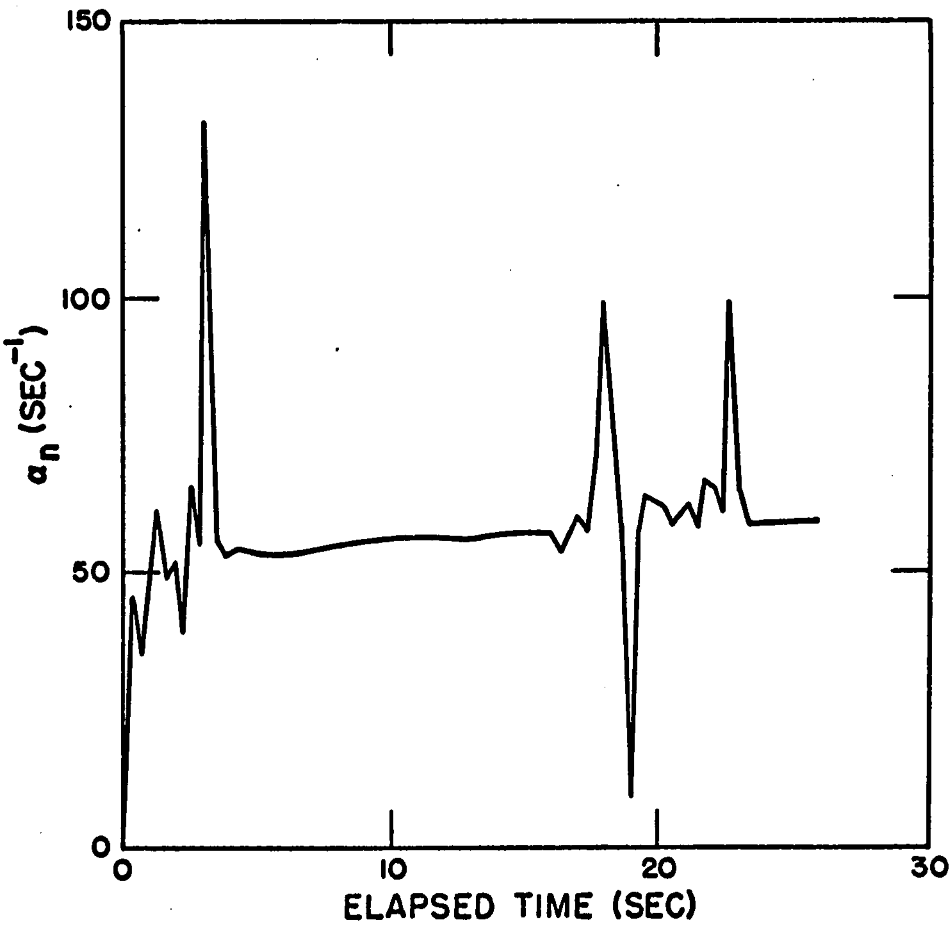

Fig. 27. Computed α_n in an Oscillating Feedback Reactor

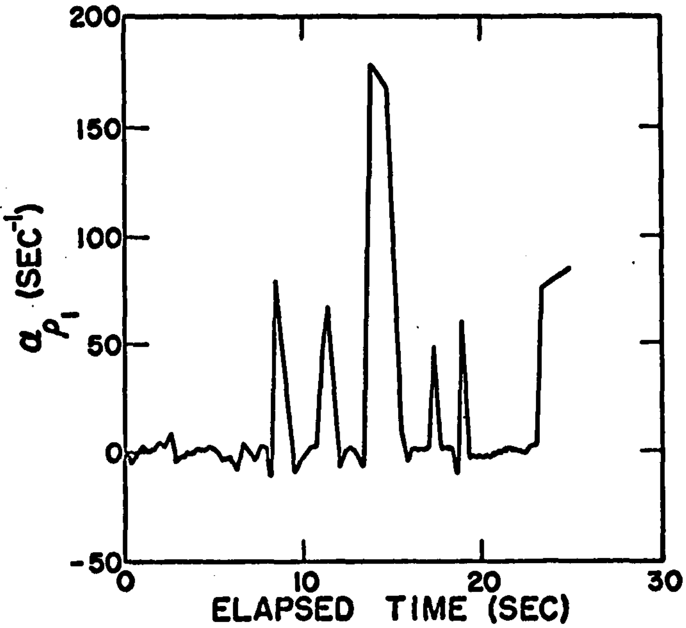

Fig. 28. Computed α_{ρ_1}

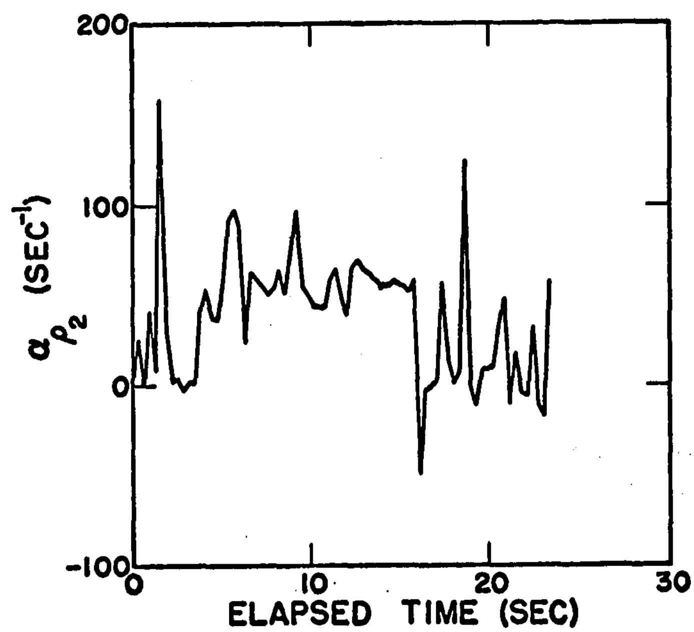

Fig. 29. Computed α_{ρ_2}

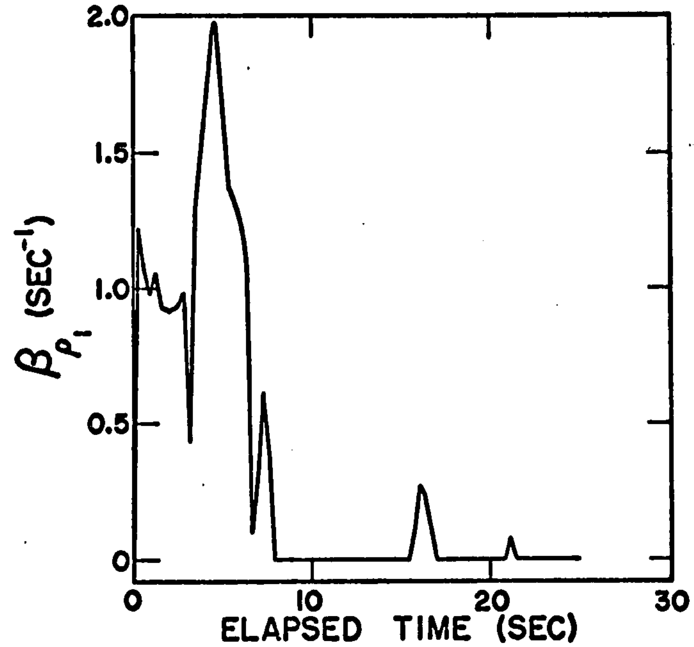

Fig. 30. Computed β_{ρ_1}

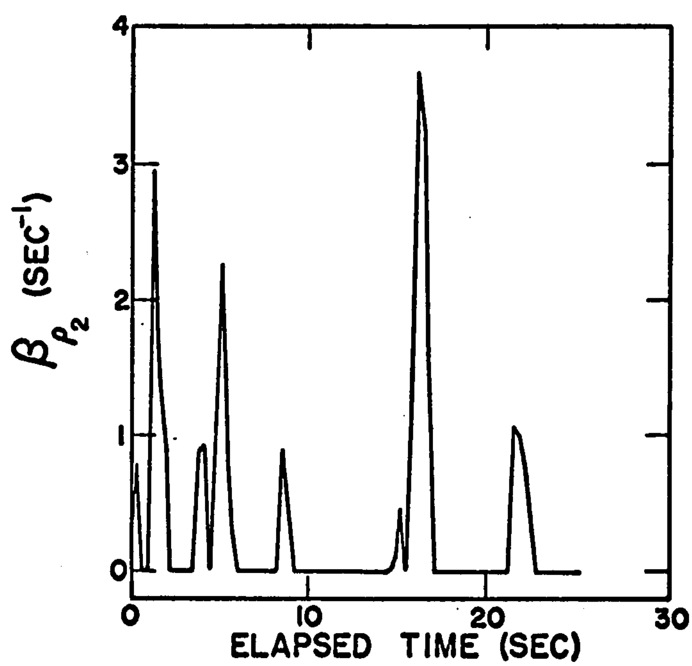

Fig. 31. Computed β_{ρ_2}

it appears, has reached a value after one cycle where the feedback reactivity $\rho_1(t)$ (Figure 25) is nearly nonoscillating. Figure 26 plots $\rho_2(t)$ and illustrates the damped oscillating behavior quite well.

Figures 27 through 31 are plots of α_n, α_{ρ_1}, α_{ρ_2}, β_{ρ_1}, and β_{ρ_2}, respectively computed using optimum integrating factors. The value of α_n is nearly everywhere equal to

$$\alpha_n = \frac{\beta_{eff} - \rho(t)}{\ell}$$

except near the beginning and end of the solution where some random variations may be observed. The variables observed in the remaining figures demonstrate quite a random behavior throughout the solution. This random behavior is attributed to the accumulated error effect during the solution. Comparisons of computer running times were made using (1) optimum integrating factors with complex exponents, (2) optimum integrating factors with real exponents, and (3) continuous analytic continuation. The results for the entire solution in each case were:

Complex = 1.12 seconds

Real = 1.31 seconds

and

Continuous Analytic Continuation = 6.47 seconds.

Despite the random behavior of these parameters, however, the complex method yielded the shortest solution time. It should be remembered that a solution using optimum integrating factors is independent of the values of α and β.

The integration step size at each position may not be maximized on the basis of the randomness observed. Smaller values of ϵ gave a more uniform appearance to the behavior of these parameters. This results because less numerical error is made in the dependent variables and their derivatives. The average solution Δt's were smaller using smaller values of ϵ, however, increasing the computer running time. It may be concluded, then, that running times are more sensitive to values of ϵ than to the degree of smoothness of α or β.

CHAPTER 4

SUMMARY AND CONCLUSIONS

A numerical integration method for obtaining the solution to coupled sets of first order nonlinear ordinary differential equations has been developed. The method, known as optimum integrating factors, is based on an integral equation solution of any ordinary differential equation where the exponent of the integrating factor is chosen to be complex. The advantages of the method over other numerical methods were investigated. Some of these advantages are: (1) an analytic criterion for the integration step size changes the step automatically depending on the behavior of the solution; (2) the advantages of other integrating factor methods are present in this method; and (3) the relative local error in the solution is at most equal to a predetermined criterion.

The method of optimum integrating factors was used to study a variety of nonlinear reactor kinetics problems. Three first order prompt neutron kinetics problems for which analytic solutions exist were investigated. Solutions by optimum integrating factors were in excellent agreement with the analytic solutions. It was determined that the error criterion was conservative--nowhere did the relative error exceed the predetermined criterion.

Three higher order delayed neutron kinetics problems for which analytic solutions are not available were also investigated. Comparisons were made of computer running times with another numerical integration method. The method of optimum integrating factors was faster in all cases. The solutions were in good agreement with predicted results. Comparisons were made of computer running times to determine the merits of using complex exponents as opposed to pure real exponents in the integrating factor. In the few cases studied the complex method was faster. It was found that the solution average integration step size is more sensitive to the magnitude of the error criterion than to the degree of smoothness of the computed inverse time constants.

It was concluded that optimum integrating factors, for the solution of reactor kinetics type problems, is a powerful numerical technique. On the basis of computer solution times, accuracy, and simplicity of problem formulation it is competitive with all of the methods now used for reactor kinetics studies.

CHAPTER 5

RECOMMENDATIONS FOR FUTURE INVESTIGATION

The power series approximation of optimum integrating factors has been investigated for order N = 3. This series utilizes the minimum amount of information required to evaluate the inverse time constants for the method. Future studies should investigate the merits of using approximating series for orders greater than three.

A number of variations of the method as programmed are conceivable. For example, after the solution has been obtained for each integration interval, new values of α and β are evaluated. Considerable savings in computer times might be achieved if these parameters were reevaluated only after Δt had changed significantly in magnitude. It was noted in the studies where analytic solutions were compared that the relative error criterion was conservative. Larger integration step sizes might be achieved if the error criterion were modified. The appropriate way in which this criterion should be modified will be investigated.

This method is presently being applied to reduce computational times of weapons calculations at the Los Alamos Scientific Laboratory. These are neutronics-hydrodynamic studies where inertia effects are studied and the prompt neutron generation times are of the order of 10^{-8} second.

Considerable savings in computational time for these studies appear to be possible.

APPENDIX A

DERIVATION OF THE INTEGRAL EQUATION

In this appendix a derivation of the basic integral equation is carried out. The solution of the first order differential equation (equation (2.2)) using a complex coefficient yields an integral equation with a real and an imaginary component. It is demonstrated here that the real part is indeed the true solution (for real dependent variables) and the imaginary part is identically zero.

The first order differential equation is

$$dy(t)/dt = -(\alpha + i\beta)y(t) + (\alpha + i\beta)y(t) + f[y(t),t] \tag{A.1}$$

and its solution is

$$\begin{aligned} y(t_j + \Delta t) = y(t_{j+1}) &= y(t_j) \exp[-(\alpha + i\beta)\Delta t] \\ &+ \exp[-(\alpha + i\beta)\Delta t]\int_0^{\Delta t} \Big\{(\alpha + i\beta)y(t_j + \tau) \\ &+ f[y(t_j + \tau), t_j + \tau]\Big\} \exp[(\alpha + i\beta)\tau]d\tau \, . \end{aligned} \tag{A.2}$$

Using the complex Euler relationships, equation (A.2) becomes

$$\begin{aligned} y(t_j + \Delta t) &= \exp(-\alpha\Delta t)[\cos \beta\Delta t - i \sin \beta\Delta t]\Big\{y(t_j) \\ &+ \int_0^{\Delta t} [(\alpha + i\beta)y(t_j + \tau) + y^{(1)}(t_j + \tau)]\exp(\alpha\tau) \\ &\times (\cos \beta\tau + i \sin \beta\tau)d\tau\Big\} \end{aligned} \tag{A.3}$$

where

$$y^{(1)}(t_j + \tau) = f[y(t_j + \tau), t_j + \tau] ,$$

Separating the real and imaginary parts of equation (A.3), and using the trigonometric identities for the sine and cosine of the difference of two angles, the following relationships are obtained:

$$\begin{aligned}\mathrm{Re}[y(t_{j+1})] = {} & y(t_j) \exp(-\alpha\Delta t) \cos \beta\Delta t \\ & + \exp(-\alpha\Delta t)\int_0^{\Delta t} [\alpha y(t_j + \tau) + y^{(1)}(t_j + \tau)] \\ & \times \exp(\alpha\tau) \cos \beta(\tau - \Delta t) d\tau - \exp(-\alpha\Delta t)\int_0^{\Delta t} \beta y(t_j + \tau) \\ & \times \exp(\alpha\tau) \sin \beta(\tau - \Delta t) d\tau \qquad \text{(A.4)}\end{aligned}$$

and

$$\begin{aligned}\mathrm{Im}[y(t_{j+1})] = {} & -y(t_j) \exp(-\alpha\Delta t) \sin \beta\Delta t \\ & + \exp(-\alpha\Delta t)\int_0^{\Delta t} [\alpha y(t_j + \tau) + y^{(1)}(t_j + \tau)] \\ & \times \exp(\alpha\tau) \sin \beta(\tau - \Delta t) d\tau \\ & + \exp(-\alpha\Delta t)\int_0^{\Delta t} \beta y(t_j + \tau) \exp(\alpha\tau) \cos \beta(\tau - \Delta t) d\tau , \qquad \text{(A.5)}\end{aligned}$$

Equations (A.4) and (A.5) may be further reduced to the following relationships:

$$\mathrm{Re}[y(t_{j+1})] = y(t_j)\ \exp\ (-\alpha\Delta t)\ \cos\ \beta\Delta t$$

$$+ \int_0^{\Delta t} \frac{d}{d\tau} \Big| \, y(t_j + \tau)\ \exp\ [\alpha(\tau - \Delta t)]$$

$$\times \cos\ \beta(\tau - \Delta t) \Big| \, d\tau \tag{A.6}$$

and

$$\mathrm{Im}[y(t_{j+1})] = -y(t_j)\ \exp\ (-\alpha\Delta t)\ \sin\ \beta\Delta t$$

$$+ \int_0^{\Delta t} \frac{d}{d\tau} \Big| \, y(t_j + \tau)\ \exp\ [\alpha(\tau - \Delta t)]\ \sin\ \beta(\tau - \Delta t) \Big| \, d\tau. \tag{A.7}$$

Finally, evaluating the integrals of equations (A.6) and (A.7), the two components are:

$$\mathrm{Re}[y(t_{j+1})] = y(t_j)\ \exp\ (-\beta\Delta t)\ \cos\ \beta\Delta t$$

$$+ y(t_j + \Delta t) - y(t_j)\ \exp\ (-\alpha\Delta t)\ \cos\ \beta(-\Delta t)$$

but,

$$\cos\ \beta(-\Delta t) = \cos\ \beta\Delta t,$$

therefore,

$$\mathrm{Re}[y(t_{j+1})] = y(t_j + \Delta t); \tag{A.8}$$

$$\mathrm{Im}[y(t_{j+1})] = -y(t_j)\ \exp\ (-\beta\Delta t)\ \sin\ \beta\Delta t$$

$$+ y(t_j + \Delta t) \times (0) - y(t_j)\ \exp\ (-\alpha\Delta t)\ \sin\ \beta(-\Delta t)$$

but,

$$\sin\ \beta(-\Delta t) = -\sin\ \beta\Delta t,$$

therefore,

$$\mathrm{Im}[y(t_{j+1})] \equiv 0\ . \tag{A.9}$$

APPENDIX B

EVALUATION OF THE $Ic_M(x)$ AND $Is_M(x)$ FUNCTIONS

Recursion formulae for the fundamental functions $Ic_M(x)$ and $Is_M(x)$ are developed in this appendix. These are integrals which must be evaluated when the dependent variable $y(t)$ and its first derivative $y^{(1)}(t)$ are expanded in Taylor series.

The definitions of these functions are

$$Ic_{M+1}(x) = \frac{e^{-\alpha x}}{M!}\int_{o}^{x} \tau^M e^{\alpha\tau} \cos \beta\tau \; d\tau \tag{B.1}$$

$$Is_{M+1}(x) = \frac{e^{-\alpha x}}{M!}\int_{o}^{x} \tau^M e^{\alpha\tau} \sin \beta\tau \; d\tau. \tag{B.2}$$

The recursion formulae are derived by integrating equations (B.1) and (B.2) by parts. For equation (B.1) let

$$u = \tau^M e^{\alpha\tau}$$

and

$$dv = \cos \beta\tau \; d\tau \cdot$$

Then

$$du = (M\tau^{M-1}e^{\alpha\tau} + \alpha\tau^M e^{\alpha\tau})d\tau$$

and

$$v = \frac{\sin \beta\tau}{\beta} ,$$

Substituting these relationships into equation (B.1) the result is

$$Ic_{M+1}(x) = \frac{x^M}{M!}\frac{\sin \beta x}{\beta} - \frac{e^{-\alpha x}}{\beta(M-1)!}\int_0^x \tau^{M-1} e^{\alpha\tau} \sin \beta\tau \; d\tau$$

$$- \frac{\alpha e^{-\alpha x}}{\beta M!}\int_0^x \tau^{M} e^{\alpha\tau} \sin \beta\tau \; d\tau$$

$$= \frac{x^M}{M!}\frac{\sin \beta x}{\beta} - \frac{Is_M(x)}{\beta} - \frac{\alpha \; Is_{M+1}(x)}{\beta} \tag{B.3}$$

Similarly, for equation (B.2) let

$$u = \tau^M e^{\alpha\tau}$$

and

$$dv = \sin \beta\tau \; d\tau ,$$

Then

$$du = (M\tau^{M-1}e^{\alpha\tau} + \alpha\tau^M e^{\alpha\tau})\, d\tau$$

and

$$v = -\frac{\cos \beta\tau}{\beta} \quad .$$

Substituting these relationships into equation (B.2) the result is

$$Is_{M+1}(x) = \frac{x^M}{m!}\frac{\cos \beta x}{\beta} + \frac{e^{-\alpha x}}{\beta(M-1)!}\int_0^x \tau^{M-1}e^{\alpha\tau}\cos \beta\tau \, d\tau$$

$$+ \frac{\alpha e^{-\alpha x}}{\beta M!}\int_0^x \tau^{M}e^{\alpha\tau}\cos \beta\tau \, d\tau$$

$$= \frac{x^M}{M!}\frac{\cos \beta x}{\beta} + \frac{Ic_M(x)}{\beta} + \frac{\alpha \, Ic_{M+1}(x)}{\beta} . \tag{B.4}$$

Substituting equation (B.4) into equation (B.3) and solving for $Ic_{M+1}(x)$ the recursion relationship is

$$Ic_{M+1}(x) = \frac{x^M}{M!}\left[\frac{\alpha \cos \beta x + \beta \sin \beta x}{\alpha^2 + \beta^2}\right]$$

$$- \frac{\beta \, Is_M(x)}{\alpha^2 + \beta^2} - \frac{\alpha \, Ic_M(x)}{\alpha^2 + \beta^2} , \tag{B.5}$$

Similarly, substituting equation (B.3) into equation (B.4) and solving for $Is_{M+1}(x)$ the recursion relationship is

$$Is_{M+1}(x) = \frac{x^M}{M!}\left[\frac{\alpha \sin \beta x - \beta \cos \beta x}{\alpha^2 + \beta^2}\right]$$

$$- \frac{\alpha \, Is_M(x)}{\alpha^2 + \beta^2} + \frac{\beta \, Ic_M(x)}{\alpha^2 + \beta^2} . \tag{B.6}$$

Equations (B.5) and (B.6) are the basic recursion formulae and may be computed easily. For M = 0 the initial functions are

$$Ic_1(x) = \frac{\alpha \cos \beta x + \beta \sin \beta x - \alpha e^{-\alpha x}}{\alpha^2 + \beta^2} \tag{B.7}$$

and

$$Is_1(x) = \frac{\alpha \sin \beta x - \beta \cos \beta x + \beta e^{-\alpha x}}{\alpha^2 + \beta^2} \quad . \tag{B.8}$$

APPENDIX C

EVALUATION OF THE F_N FUNCTIONS

Equation (2.10) in the text is the defining equation for the terminal coefficient of the approximating power series. Restated, this coefficient is

$$F_N(\alpha,\beta,\Delta t) = Ic_N(\Delta t)\cos\beta\Delta t + Is_N(\Delta t)\sin\beta\Delta t\ . \qquad (C.1)$$

Utilizing the definitions of $Ic_N(\Delta t)$ and $Is_N(\Delta t)$, equation (C.1) becomes

$$F_N(\alpha,\beta,\Delta t) = \frac{e^{-\alpha\Delta t}}{(N-1)!}\int_o^{\Delta t} \tau^{N-1}e^{\alpha\tau}(\cos\beta\tau\cos\beta\Delta t$$

$$+ \sin\beta\tau\sin\beta\Delta t)d\tau$$

$$= \frac{1}{(N-1)!}\int_o^{\Delta t} \tau^{N-1}e^{\alpha(\tau-\Delta t)}\cos\beta(\tau - \Delta t)d\tau\ . \qquad (C.2)$$

Recalling the infinite series expansion for $\exp(\alpha x)\cos\beta x$

$$\exp(\alpha x)\cos\beta x = \sum_{k=o}^{\infty}\frac{c_k}{k!}x^k\ , \qquad (C.3)$$

the series for F_N then becomes

$$F_N(\alpha,\beta,\Delta t) = \frac{1}{(N-1)!}\sum_{k=o}^{\infty}\frac{c_k}{k!}\int_o^{\Delta t}\tau^{N-1}(\tau - \Delta t)^k d\tau \; . \qquad (C.4)$$

Performing the integration for all k the result, required for equation (2.15) in the text, is

$$F_N(\alpha,\beta,\Delta t) = \sum_{k=o}^{\infty}\frac{c_k \Delta t^{N+k}}{(N+k)!} \; , \qquad (C.5)$$

APPENDIX D

DERIVATION OF THE EXPRESSION FOR THE RELATIVE TRUNCATION ERROR

The relative truncation error for the approximating series of $y(t)$ was given for order N in equation (2.17) of the text as

$$\sum_{k=o}^{\infty} \frac{\Delta t^{N+k}}{(N+k+1)!} \left| \frac{c_k \delta y^{(N)} - c_{k+1} \delta y^{(N-1)}}{y(t_{j+1})} \right| \leq \epsilon \quad . \tag{D.1}$$

To a first approximation, it will be demonstrated in this appendix that

$$c_k \delta y^{(N)} - c_{k+1} \delta y^{(N-1)} = c_k \left[(\alpha^2 + \beta^2) \delta y^{(N-2)} + 2\alpha \delta y^{(N-1)} + \delta y^{(N)} \right] . \tag{D.2}$$

To do so, information concerning the truncation error for the approximating series of order (N-1) is used. This relationship will be set identically zero.

$$\sum_{k=o}^{\infty} \frac{\Delta t^{N+k-1}}{(N+k)!} \left| \frac{c_k \delta y^{(N-1)} - c_{k+1} \delta y^{(N-2)}}{y(t_{j+1})} \right| = 0 \tag{D.3}$$

This equation is valid if each term of the series is zero.

Observing equation (D.2), eliminating $c_k \delta y^{(N)}$ from both sides

$$c_k \delta y^{(N-2)} + \frac{(2\alpha c_k + c_{k+1})}{\alpha^2 + \beta^2} \delta y^{(N-1)} = 0 \ . \tag{D.4}$$

Using the recursive relationships for c_k and s_k it can be shown that the coefficient of $\delta y^{(N-1)}$ is $-c_{k-1}$.

$$c_k = -\alpha c_{k-1} - \beta s_{k-1} \tag{D.5}$$

$$s_k = \beta c_{k-1} - \alpha s_{k-1} \tag{D.6}$$

and

$$\begin{aligned} c_{k+1} &= -\alpha c_k - \beta s_k \\ &= (\alpha^2 - \beta^2) c_{k-1} + 2\alpha\beta s_{k-1} \ , \end{aligned} \tag{D.7}$$

Using equations (D.5) and (D.7)

$$\begin{aligned} \frac{(2\alpha c_k + c_{k+1})}{\alpha^2 + \beta^2} &= \frac{-2\alpha^2 c_{k-1} - 2\alpha\beta s_{k-1} + (\alpha^2 - \beta^2) c_{k-1} + 2\alpha\beta s_{k-1}}{\alpha^2 + \beta^2} \\ &= -c_{k-1} \ , \end{aligned} \tag{D.8}$$

Substituting equation (D.8) into equation (D.4) the result is

$$c_k \delta y^{(N-2)} - c_{k-1} \delta y^{(N-1)} = 0 \ . \tag{D.9}$$

If equation (D.3) is true for all k, which is a first approximation to the error, then if k is replaced by k+1 equation (D.9) is still valid. This, then, is the criterion which must be satisfied regardless of the value of k for equation (D.3) to hold.

To a first approximation, therefore, the error criterion of equation (D.1) is

$$\left| \frac{(\alpha^2 + \beta^2)\delta y^{(N-2)} + 2\alpha\delta y^{(N-1)} + \delta y^{(N)}}{y(t_{j+1})} \right| \sum_{k=o}^{\infty} \frac{c_k \Delta t^{N+k}}{(N+k+1)!} \leq \epsilon \; . \qquad \text{(D.10)}$$

APPENDIX E

COMPUTER LISTING OF THE NUMERICAL

INTEGRATION SUBROUTINE

```
      SUBROUTINE TYME
      COMMON /DTN/DT1,DT2,DT3,DT4
      COMMON A      , COM    , N
      COMMON /NNP/NP
      DIMENSION A(4300),COM(15000),N(280)
      DIMENSION Y(120),YP(120),Y2(120),Y3(120),YO(120)
     1,YP1(120),YP2(120),YP3(120),AL(120),BT(120)
      DIMENSION C(250),Z(500)
      EQUIVALENCE (A(1),Z),(A(501),C)
      EQUIVALENCE (A(901),Y),(A(1021),YP),(A(1141),Y2)
     1,(A(1261),Y3),(A(1381),YO),(A(1501),YP1),(A(1621)
     2,YP2),(A(1741),YP3),(A(1861),AL),(A(1981),BT),(A(871)
     3,T),(A(872),DT),(A(874),TS),(A(875),TSTOP),(A(877)
     4,TEST),(N(4),ITIME),(N(7),NV),(N(257),IDT)
C   SUBROUTINE TYME MAY BE USED TO SOLVE AS MANY AS 120
C   DIFFERENTIAL EQUATIONS SIMULTANEOUSLY USING THE METHODS
C   OF OPTIMUM INTEGRATING FACTORS OR CONTINUOUS ANALYTIC
C   CONTINUATION.  TEN STORAGE LOCATIONS ARE REQUIRED FOR
C   EACH ODE.  TEST=THE ERROR CRITERION.  ITIME=INTEGRATION
C   SCHEME OPTION.  NV=NUMBER OF DIFFERENTIAL EQUATIONS.
C   T=INDEPENDENT VARIABLE.  TS=INITIAL VALUE OF T.  TSTOP=
C   FINAL VALUE OF T.  DT1=COMPUTED INTEGRATION STEP SIZE.
C   DT=MAXIMUM ALLOWABLE INTEGRATION STEP SIZE.  IF IDT=0
C   A PRINT OUT IS MADE AFTER EACH DT INTERVAL--IF IDT=1
C   A PRINT OUT IS MADE AFTER EVERY INTEGRATION INTERVAL.
C   TO START THE PROBLEM SPECIFY ALL INITIAL CONDITIONS FOR
C   Y (DEPENDENT VARIABLES).  YP=FIRST DERIVATIVE, Y2=SECOND
C   DERIVATIVE, Y3=THIRD DERIVATIVE.  SUBROUTINE STARTI(TEST)
C   DETERMINES INITIAL DT1.  SUBROUTINE DER CONTAINS ALL
C   DERIVATIVE EQUATIONS.
      F=0
      C10=24.*TEST
      IF(IDT.EQ.1)DT=TSTOP-T
      TPR=T+DT
      IF(NP.GT.0)GO TO 1
      CALL STARTI(TEST)
      DT3=0.
      NP=1
    1 T1=T
      F=F+1.
```

```
      DO 12 I=1,NV
      DY=Y(I)-YO(I)
      DY1=YP(I)-YP1(I)
      DY2=Y2(I)-YP2(I)
      DY3=Y3(I)-YP3(I)
      AL(I)=0.
      BT(I)=0.
      IF(ITIME.EQ.6)GO TO 3
      IF(DY2.NE.0.)AL(I)=-DY3/DY2
      IF(ITIME.EQ.7)GO TO 3
      WN=DY3*DY1-DY2**2
      WD=DY2*DY -DY1**2
      IF(WD*WN.LE.0..OR.DY2.EQ.0.)GO TO 3
      W2=WN/WD
      ZT=-(DY3+W2*DY1)/2./DY2
      IF(ZT*ZT.GT.W2)GO TO 3
      AL(I)=ZT
      BT(I)=SQRT(W2-ZT*ZT)
    3 IF(AL(I)*DT1.LT.-4.)DT1=4./ABS(AL(I))
   12 CONTINUE
      INIT=0
    2 IF(T1+DT1.GT.TPR)DT1=TPR-T1
      T=T1+DT1
      INIT=INIT+1
      DT5=DT
      DO 8 I=1,NV
      DY1=YP(I)-YP1(I)
      DY2=Y2(I)-YP2(I)
      DY3=Y3(I)-YP3(I)
      IF(INIT.GT.1)GO TO 4
      YO(I)=Y(I)
      YP1(I)=YP(I)
      YP2(I)=Y2(I)
      YP3(I)=Y3(I)
    4 AD=DT1*AL(I)
      BD=DT1*BT(I)
      E=0.
      IF(AD.LT.700.)E=EXP(-AD)
      A2=AL(I)**2
      B2=BT(I)**2
      W2=A2+B2
      C8=C10
      C9=DY3
      F1=DT1
      F2=F1*DT1/2.
      F3=F2*DT1/3.
      IF(W2.EQ.0.)GO TO 7
      IF(B2.NE.0.)GO TO 6
      CD=AD-1.+E
```

```
      F3=(AD*AD/2.-CD)/(A2*AL(I))
      C8=C8*ABS(1.+AD/5.)
      C9=AL(I)*DY2+C9
      GO TO 7
    6 IF(A2.EQ.0.)GO TO 10
      F3=(AD*AD/2.+(B2-A2)*AD/W2+A2*(A2-3.*B2)/W2/W2/
     1(AL(I)*W2)+E*(COS(BD)* AL(I)*(3.*B2-A2)+BT(I)*
     2(3.*A2-B2)*SIN(BD))/W2/W2/W2
      C8=C8*ABS(1.+2.*AD/5.+W2*DT1**2/30.)
      C9=W2*DY1+2.*AL(I)*DY2+C9
      GO TO 7
   10 F3=(BD-SIN(BD))/(BT(I)*B2)
      C8=C8*ABS(1.+BD*BD/30.)
      C9=B2*DY1+C9
    7 Y(I)=YO(I)+F1*YP1(I)+F2*YP2(I)+F3*YP3(I)
      C8=C8*ABS(Y(I))
      C9=ABS(C9)
      IF(C9*DT5**3.LT.C8)GO TO 5
      DT5=(C8/C9)**(1./3.)
    5 IF(AL(I)*DT5.LT.-4.)DT5=4./ABS(AL(I))
    8 CONTINUE
      CALL DER
      IF(INIT.EQ.1)GO TO 2
      IF(DT5.GT.DT1*.5)GO TO 9
      IF(INIT.GT.10) GO TO 11
      DT1=DT5
      GO TO 2
    9 DT1=DT5
      IF(IDT.EQ.1)RETURN
      IF(T.LT.TPR)GO TO 1
      DTAV=DT/F
      WRITE(6,1002)DTAV
 1002 FORMAT(6H DTAV=,E10.3)
   11 WRITE(6,1003)INIT,TEST ,T,DT1
 1003 FORMAT(23H DT DID NOT CONVERGE IN,I4,21H PASSES FOR
     1CRITERION, E10.3,/7H TIME=,E10.3,6X,6HDT1 = ,E10.3)
      CALL EXIT
 1000 RETURN
      END
```

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