91-102
LA-6483-MS

Informal Report

UC-32 and UC-34

Reporting Date: August 1976

Issued: September 1976

42-424

The Calculation of Isotopic Mass and Energy Production by a Matrix Operator Method

by

Clarence E. Lee

los alamos
scientific laboratory
of the University of California
LOS ALAMOS, NEW MEXICO 87545

An Affirmative Action/Equal Opportunity Employer

MASTER

Printed in the United States of America. Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road
Springfield, VA 22161
Price: Printed Copy \$3.50 Microfiche \$2.25

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Energy Research and Development Administration, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights.

THE CALCULATION OF ISOTOPIC MASS AND ENERGY PRODUCTION BY A MATRIX OPERATOR METHOD

by

Clarence E. Lee

ABSTRACT

The Volterra method of the multiplicative integral is used to determine the isotopic density, mass, and energy production in linear systems. The solution method, assumptions, and limitations are discussed. The method allows a rapid accurate calculation of the change in isotopic density, mass, and energy production independent of the magnitude of the time steps, production or decay rates, or flux levels.

NOTICE
This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Energy Research and Development Administration, nor any of their employees, nor any of their contractors, subcontractors, or their employees, make any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights.

I. INTRODUCTION

Numerous approximate techniques have been developed over the last two decades to solve the problem of an accurate calculation of isotope and energy production and decay in linear systems. These methods are not reviewed here at this time.

We summarize a calculational technique based on the calculus of Volterra involving the multiplicative integral.¹ This technique allows a rapid accurate calculation of the change in density and energy production rate independent of the magnitude of the time constants, decay rates, or flux levels. The method has been applied successfully in a number of problems² and unpublished codes.

II. BALANCE EQUATION

Let $N_i(\underline{r}, t)$ be the nuclear density of the i^{th} isotope in a general transmutation chain at position $\underline{r}$ and time t in a system with neutron flux $\phi(\underline{r}, E, t)$ having energy between E and $E + dE$. No processes involving neutrons as initial

or final products need be excluded, although their effects must be approximated in order to achieve a linear system of equations. The balance equation, including production and decay, is given by²

$$\frac{\partial N_i(r, t)}{\partial t} = Q_i(r, t) - \lambda_i(r) N_i(r, t) + \sum_j \lambda_{ij}(r) N_j(r, t) + \int_0^\infty dE' \left[-\sigma_i^a(r, E', t) N_i(r, t) + \sum_j \sigma_{ij}^a(r, E', t) N_j(r, t) \right] \phi(r, E', t), \quad (1)$$

where λ_i is the decay constant of the i^{th} isotope, λ_{ij} is the decay of isotope j to i , σ_i^a is the absorption cross section for conversion of isotope j to i for example by (n, α) , $(n, 2n)$, etc.-and ϕ is the neutron flux. A general source-sink term is included, but for the purposes of this report will not be treated in detail.

III. MATRIX OPERATOR SOLUTION

Equation (1) may be written in matrix form by letting N_i and Q_i be elements of a column vector. The spatial dependence is implicit. Defining the elements of a matrix S by

$$S_{ii}(t) = -\lambda_i - \int_0^\infty dE' \sigma_i^a(E', t) : (E', t) \quad (2)$$

$$S_{ij}(t) = \lambda_{ij} + \int_0^\infty dE' \sigma_{ij}^a(E', t) : (E', t),$$

then Eq. (1) takes the form

$$\frac{\partial \underline{N}(t)}{\partial t} = \underline{Q}(t) + \underline{S}(t) \underline{N}(t). \quad (3)$$

Following Ref. 1, if we define the matricant $\phi_{t_0}^t(S)$ by *

$$\phi_{t_0}^t(S) = I + \int_{t_0}^t S(t) dt + \int_{t_0}^t dt S(t) \int_{t_0}^t d\sigma S(\sigma) + \dots, \quad (4)$$

that converges absolutely and uniformly in every closed interval in which $S(t)$ is continuous, we may write the solution

* I is the identity matrix

$$\underline{N}(t) = \underline{\Lambda}_t^t(S) \underline{N}(t_0) + \int_{t_0}^t d\tau \underline{K}_t(t, \tau) \underline{Q}(\tau), \quad (5)$$

where

$$\underline{K}_t(t, \tau) = \underline{\Lambda}_t^t(S) \left[\underline{\Lambda}_\tau^t(S) \right]^{-1}. \quad (6)$$

Dividing the interval (t_0, t) into n parts by introducing the intermediate points t_i ($1 \leq i \leq n-1$) and setting $\Delta t_k = t_k - t_{k-1}$ for $1 \leq k \leq n$ with $t = t_n$ and $t_0 = t_0$, it is readily shown that

$$\underline{\Lambda}_t^t(S) = \lim_{\Delta t_k \rightarrow 0} \left[e^{S(t_n) \Delta t_n} \dots e^{S(t_2) \Delta t_2} e^{S(t_1) \Delta t_1} \right]. \quad (7)$$

The various values of the matrix function $S(t)$ are, in general, not permutable in the time subintervals Δt_k . In the very special case in which they are permutable, namely

$$\left(S(t'), S(t'') \right) = S(t')S(t'') - S(t'')S(t') = 0, \quad (8)$$

for $t', t'' \in (t_0, t)$, then Eq. (7) becomes

$$\underline{\Lambda}_t^t(S) = \exp \left[\int_{t_0}^t d\tau S(\tau) \right]. \quad (9)$$

For example, if $S(t') = \text{constant}$ for $t' \in (t_0, t)$, then Eq. (8) is satisfied and substitution of Eqs. (5) and (6) yields the solution

$$\underline{N}(t) = e^{S(t-t_0)} \underline{N}(t_0) + e^{\int_{t_0}^t d\tau S(\tau-t_0)} \underline{Q}(\tau). \quad (10)$$

This solution is valid for the frequently made assumption that the flux is constant in a time interval (t_0, t) .

Several other obvious functional forms may be considered.

$$(1) \text{ Suppose } S(t') = S_0 \int_{t_0}^{t'} dt' f(t'). \quad (11)$$

The solution in this case is just Eq. (10) with the replacement

$$S_0 \int_{t_0}^t dt' f(t') \rightarrow S. \quad (12)$$

Returning to Eqs. (1) and (2) it is clear that this approximation requires that $\lambda_{ij} = \lambda_{ji} = 0$ for all i, j . Physically this means that the dominant behavior of the solution is from absorption and conversion with decay being negligible. If decay is the dominant process ($f(t') = 0$ or $f(t') \approx \text{constant}$), so that $S(t')$ is constant, then Eq. (10) is the solution. If both decay and conversion are important we may use the mean value theorem to define

$$\bar{f} = \int_{t_0}^t dt' f(t') / (t - t_0) \quad (13)$$

and approximate the matrix elements of Eq. (2) by their averaged values in the interval (t_0, t) .

(2) Suppose $S(t') = S_0 + S_1 f(t')$, where S_0 and S_1 are constant for $t' \in (t_0, t)$. This is the form that Eq. (2) takes if the spectral effects separate in energy and time. Clearly Eq. (8) is not satisfied unless either $(S_0, S_1) = 0$ or $f(t'') = f(t')$ for all $t', t'' \in (t_0, t)$. If $f(t'') = f(t')$, then $f(t') = \text{constant}$ and the solution is given by Eq. (10). If we consider the case $(S_0, S_1) \neq 0$ it seems not to be generally true unless either S_0 or S_1 is a constant times the identity matrix.

This case is also the form encountered in kinetics problems and thus, Eq. (10) is not a possible solution form unless $f(t) = \text{constant}$, notwithstanding its usage in the literature which is open to criticism except as a crude approximation. For problems in which $S(t') = S_0 + S_1 f(t')$ cannot be adequately approximated using the mean value theorem technique described previously, a solution using Laplace transform techniques would seem to be a successful approach.

IV. EIGENVALUES

The matrix elements of S are given by Eq. (2). We note that the diagonal elements are negative and the off-diagonal elements are nonnegative since the mean lifetimes and cross sections are intrinsically nonnegative. Further, since the λ_{ij} represent partial inverse mean lifetimes for spontaneous decay from isotope j to i , we have the constraint

$$\lambda_j \geq \sum_i \lambda_{ij}, \quad (14)$$

where the inequality obtains whenever some possible process is omitted from the chain equations. Similarly, since σ_{ij} represents the transmutation cross section from isotope j to i , we have

$$\sigma_j^a \geq \sum_i \sigma_{ij} \quad , \quad (15)$$

since σ_j^a cannot otherwise represent the total absorption crosssection by the processes being considered. Thus, using Eqs. (14) and (15) in Eq. (2) we conclude that

$$|S_{ii}| \geq \sum_j' |S_{ji}| \quad , \quad (16)$$

where the prime on the summation indicates that the term $i=j$ is excluded. But Eq. (16) is just the statement that S is nonnegative.

From the Levy-Hadamard-Gerschgorin theorems,³ the eigenvalues of S lie inside the closed domain G consisting of all circles K_i ($i = 1, 2, \dots$) with centers at S_{ii} and radii r_i , where

$$r_i = \sum_{j \neq i} |S_{ji}|. \quad (17)$$

We have used the theorem in its transposed form. Since Eq. (16) is satisfied, we conclude that all the centers are on the negative real axis (since all the S_{ii} are real and negative), and that all the eigenvalues of S have negative real parts.

If the matrix S is triangular it is easily shown that all the eigenvalues given by Eq. (2) are real and negative. In fact they are just S_{ii} . The matrix S would be triangular, for example, if there were no contributions to an isotope in a chain from an isotope beyond that point in the chain. This would exclude $(n, \gamma) + \beta^-$, $(n, 2n)$ reactions unless additional approximations were made. Although chains leading to a triangular S matrix certainly exist, not all chains of interest have this property. For this calculation we prefer therefore not to introduce these unnecessary approximations in order to make S triangular. A general and computationally rapid solution can be obtained for S nontriangular.

V. SOLUTION METHOD

In this report we limit our discussion to the cases for which $S(t')$ is constant or $S(t') = S_0 f(t')$ for $t' \in (t_0, t)$. Initially we assume $Q = 0$, and then give the solution for $Q(t') = \text{constant}$. Then Eq. (10) reduces to the simple form

$$\underline{N}(t) = e^{S(t-t_0)} \underline{N}(t_0), \quad (18)$$

where the matrix operator $e^{S\tau}$ is defined by¹

$$e^{S\tau} = \sum_{k=0}^{\infty} \frac{(S\tau)^k}{k!}, \quad (19)$$

which is exactly the result obtained from evaluating the matricant $M_0^{\tau}(S)$ in Eq. (4) provided Eq. (8) is satisfied.

Since S has eigenvalues with negative real parts, it is trivially true that $e^{S\tau}$ is nonnegative* and has eigenvalues

$$\mu(e^{S\tau}) = e^{-\Lambda \pm i\Gamma}, \quad (20)$$

where Λ and Γ are the real and imaginary parts of the eigenvalues of $S\tau$. Hence,

$$0 \leq |\mu| \leq 1. \quad (21)$$

We now consider the explicit evaluation of $e^{S\tau}$. Although by Eq. (21) the magnitude of the eigenvalues of $e^{S\tau}$ are bounded by unity, and Eq. (19) is uniformly and absolutely convergent, the direct usage of Eq. (19) for cases such that $\|S\tau\| \gg 1$ can lead to a computational catastrophe.

We may rewrite Eq. (18) as

$$\underline{N}(t) = \underline{N}(t_0) + C D(C) \underline{N}(t_0), \quad (22)$$

which is an identity if $C = S(t - t_0)$, and we define

$$D(C) = C^{-1}(e^C - I) = \sum_{k=0}^{\infty} \frac{C^k}{(k+1)!}. \quad (23)$$

Clearly the matrix $D(C)$ exists even if C is singular.** Although the eigenvalues of μ , Eq. (20), are bounded by unity, and the eigenvalues of C are bounded, the

* If $S_{ij} > 0$ for $i \neq j$, $e^{S\tau} = I + S\tau + \dots$ is nonnegative

**For example, for a decay scheme involving a stable isotope, C is singular.

fact that the eigenvalues of $C, (\lambda + i\tau)\tau$, are not necessarily bounded by unity is what causes the difficulty in evaluating Eq. (19) or (23) directly.

Using the laws of exponentiation⁴ we may readily scale the matrix C until its eigenvalues are bounded by unity and then compute $e^{S\tau}$ using a recursion relationship to scale back up to $S\tau$.

If we define the matrix H by

$$H = 2^{-p}C \quad (24)$$

to have eigenvalues less than unity, then we may determine³ p from

$$2^p = \max_{i,j} |C_{ij}|^2 \quad (25)$$

or

$$p > \ln(\max_{i,j} |C_{ij}|^2) / \ln 2, \quad (26)$$

where $\ln$ is the natural logarithm. Now from Eq. (23)

$$D(H) = H^{-1}(e^H - I). \quad (27)$$

We now derive and prove the recursion relationship by induction. If $p = 0$

$$D(H) = D(C). \quad (28)$$

If $p = 1$, then since $(H, H) = 0$, we may write

$$\begin{aligned} D(C) &= D(2H) \\ &= (2H)^{-1}(e^{2H} - I) \\ &= H^{-1}(e^H - I) \frac{1}{2}(e^H + I) \\ &= D(H) (I + \frac{1}{2}HD(H)). \end{aligned} \quad (29)$$

Now, by induction we may write

$$\begin{aligned} D(2^p H) &= D(2^{p-1} H) (I + \frac{1}{2}(2^{p-1} H)D(2^{p-1} H)) \\ &= D(C). \end{aligned} \quad (30)$$

For suppose Eq. (30), which is true for $p = 0, 1$, is true for $p = n$, then let us evaluate $D(2^{n+1} H)$ as

$$\begin{aligned} D(2^{n+1} H) &= (2^{n+1} H)^{-1}(e^{2^{n+1} H} - I) \\ &= (2^n H)^{-1}(e^{2^n H} - I) \frac{1}{2}(e^{2^n H} + I) \\ &= D(2^n H) (I + \frac{1}{2}(2^n H)D(2^n H)), \end{aligned} \quad (31)$$

we have only used Eq. (31) and $(H, H) = 0$. Therefore, since Eq. (30) has same form as Eq. (31), by transfinite induction it is true for all $p \geq 0$.

The evaluation of the matrix $D(H)$ is approximated, of course, by a finite number of terms. We denote this approximation by

$$D^M(H) = \sum_{k=0}^M \frac{H^k}{(k+1)!} \approx H^{-1}(e^H - I) \quad (32)$$

and evaluate it as a factored matrix polynomial

$$D^M(H) = H(I + \frac{H}{2}(I + \dots (\dots \frac{H}{M-2}(I + \frac{H}{M-1}(I + \frac{H}{M}) \dots))) \quad (33)$$

from the M^{th} term backwards, where M is a suitably chosen integer. If we assume that $\|H\| < \frac{1}{2}$, then the first term omitted contributes an error, E_M , of order

$$E_M = \frac{\|H\|^{M+1}}{(M+2)!} < \frac{1}{2^{M+1}(M+2)!} \quad (34)$$

In Table I we give representative values of E_M versus M .

TABLE

E_M ERROR CONTRIBUTIONS TO $D(H)$ FOR $M + 1^{\text{st}}$ TERM OMITTED

M	E_M	M	E_M
1	4.17×10^{-2}	9	2.45×10^{-11}
2	5.21×10^{-3}	10	1.02×10^{-12}
3	5.21×10^{-4}	11	3.92×10^{-14}
4	4.34×10^{-5}	12	1.40×10^{-15}
5	3.10×10^{-6}	13	4.67×10^{-17}
6	1.94×10^{-7}	14	1.46×10^{-18}
7	1.08×10^{-8}	15	4.29×10^{-20}
8	5.38×10^{-10}	20	4.24×10^{-28}

VI. COMPARISON WITH LINEAR METHOD

It is of interest to compare the relative computation times of this method with those of the linear methods ($M = 1$, $p = 0$) frequently used. If the elements of the matrix S_T in Eq. (19) satisfy the requisite accuracy criteria in Eq. (34) with $M = 1$ and $p = 0$, then it is a simple matter to arrange the computer subroutine to run this case as efficiently as the linear methods. This we assume to be the case.

However, if $M > 1$ and/or $p > 0$ is required, then for the same overall accuracy the linear method would have to run with a smaller time step.

Let $\alpha = ||S_T||$ as defined in Eq. (25), say. Then for the accuracy given by Eq. (34), the linear method needs n steps determined by

$$\frac{\alpha^n}{n} \leq E_M. \quad (35)$$

Using the matrix operator method, we subdivide α into p intervals, determined by

$$p \geq \max \left(1, \left[\frac{\ln \alpha}{\ln 2} \right] + 1 \right), \quad (36)$$

where $[] \equiv$ least integer and determine M from Eq. (34) for a specified accuracy E_M . Designate X as the time for a computer matrix multiply and Y for a matrix add. Then the linear method requires $X + Y$ matrix operation times, and the matrix operator method requires $(3p + M)X + (p + M)Y$ operation times. Assuming that $X = 5Y$, as is usually the case, and using Eq. (35) - (36), we find the ratio of the linear to the matrix operator times, R , to be given by

$$R = \frac{3\alpha 2^{M+1} (M+2)!}{(8p + 3M)}. \quad (37)$$

Equation (37) is evaluated for various α and M in Table II. It is clear that the matrix operator method is superior to the linear method for $\alpha > 10^{-2}$ and $M \geq 2$. This will occur whenever high fluxes, long times, or short lifetimes enter. The matrix operator method is always as fast as the linear method by construction. In complex problems it is superior.

Explicit integration techniques (Runge-Kutta, and others) follow directly from terminating the matricant $\Omega_{t_0}^t(S)$, Eq. (4), at some level and then applying

TABLE II
RATIO R OF THE LINEAR TO MATRIX OPERATOR COMPUTING TIMES

$\frac{a}{M}$	10^{-6}	10^{-3}	10^{-2}	10^{-1}	1	10	10^2	10^3	10^4
1	1.	1.	1.	2.4	6.5	20.6	122	867	6.3×10^3
2	1.	1.	1.	9.6	41.1	152	929	6.7×10^3	4.9×10^4
3	1.	1.	6.4	64	339	1.4×10^3	8.9×10^3	6.5×10^4	4.8×10^5
4	1.	5.8	57.6	576	3.5×10^3	1.6×10^4	1.0×10^5	7.5×10^5	5.6×10^6
5	6.5	64.5	645	6.5×10^3	4.2×10^4	2.1×10^5	1.4×10^6	1.0×10^7	7.6×10^7
6	86	860	8.6×10^3	8.6×10^4	6×10^5	3.1×10^6	2.1×10^7	1.6×10^8	1.2×10^9
7	1.3×10^3	1.3×10^4	1.3×10^5	1.3×10^6	9.6×10^6	5.3×10^7	3.6×10^8	2.8×10^9	2.1×10^{10}
8	2.3×10^4	2.3×10^5	2.3×10^6	2.3×10^7	1.7×10^8	1.0×10^9	7.0×10^9	5.4×10^{10}	4.1×10^{11}
9	4.5×10^5	4.5×10^6	4.5×10^7	4.5×10^8	3.5×10^9	2.1×10^{10}	1.5×10^{11}	1.1×10^{12}	8.8×10^{12}
10	9.8×10^6	9.8×10^7	9.8×10^8	9.8×10^9	7.7×10^{10}	4.7×10^{11}	3.4×10^{12}	2.7×10^{13}	2.1×10^{14}

Eq. (7) with a suitably small Ωt_k . Since the matrix has eigenvalues with negative real parts, the errors made by these approximations decay.

VII. TIME REVERSAL

One might expect that an arbitrary final condition could be specified and the corresponding initial state could be computed,⁴ given the matrix $S\tau$. This is, in fact, not the case. The reason may be expressed in several different ways: (1) Loss of significance, or equivalently, entropy gain, and one finds an infinite class of equivalent initial conditions yielding the same final state. Many have negative, albeit small, initial densities. (2) Reversing the time sign changes the sign of the real part of the eigenvalues from negative to positive. By the Liapunov Theorems,¹ the solutions then become unstable and one should not expect to achieve accurate time-reversed solutions.

For small $S\tau$ elements one can achieve an approximate time-reversed solution, but for $||S\tau|| \geq 2$, these solutions become very inaccurate.

VIII. SOLUTION FOR CONSTANT SOURCE Q

Returning to Eq. (10) when $Q(t) \neq 0$, let us assume $Q(t') = Q_0 = \text{constant}$ for $t' \in (t_0, t)$. Substituting this assumption into Eq. (10) and using Eqs. (22) and (23), we find

$$\underline{N}(t) = e^{S(t - t_0)} \underline{N}(t_0) + S^{-1}(e^{S(t - t_0)} - 1) \underline{Q}_0 \quad (38)$$

or

$$\underline{N}(t) = \underline{N}(t_0) + CD(C)\underline{N}(t_0) + (t - t_0)D(C)\underline{Q}_0, \quad (39)$$

where

$$C = S(t - t_0) \quad (40)$$

and $D(C)$ is given by Eq. (23).

IX. ENERGY PRODUCTION

We are also interested in determining the energy release resulting from Eq. (1) in a given material as a result of fission, (n, γ) , $(n, 2n)$, β^- decay, etc., such as would occur in a reactor in steady state or transient operation, or in a star.

Let K_r be the energy released or absorbed for the r^{th} reaction, which is determinable from the mass defect. In Eq. (10) we may write the matrix S as

$$S_{ij} = B_{ij}^r \otimes I_r, \quad (41)$$

where B_{ij}^r is the $\phi\sigma$ for the r^{th} reaction, I_r is an r -dimensional unit vector, and $\otimes$ is the Cartesian product. The summation convention on repeated indices is used. In this notation the energy matrix, F , takes the form

$$F_{ij} = B_{ij}^r \otimes K_r. \quad (42)$$

Using Eq. (42) the energy production rate dE/dt from M grams of material is given by

$$\frac{dE(t)}{dt} = F A^{-1} \underline{M}(t), \quad (43)$$

where A is the diagonal atomic mass matrix, $\underline{M}$ is the isotopic mass vector, and dE/dt is the energy production rate vector with an entry for each isotopic constituent involved in the chain under consideration. The mass vector is defined in term of the density vector by

$$\underline{M}(t) = A \underline{N}(t). \quad (44)$$

Hence, for $Q(t') = 0$, $\underline{M}(t)$ is given from Eq. (18) as

$$\underline{M}(t) = A e^{\int_0^t ds S(s)} A^{-1} \underline{M}(t_0), \quad (45)$$

where we have assumed $S(s)$ is of the form that Eq. (9) is valid.

Substituting Eqs. (45) and (18) into (43) and integrating we obtain

$$\underline{E}(t) - \underline{E}(t_0) = F W(t) A^{-1} \underline{M}(t_0), \quad (46)$$

where

$$W(t) = \int_0^t ds e^{\int_0^s ds' S(s')}. \quad (47)$$

Assuming the constant flux approximation, $S = S_0$ in Eq. (47), we obtain

$$W_C(t) = \int_0^t ds e^{S_0 \tau} = \tau D(S_0 \tau), \quad (48)$$

where $D(S_0 \tau)$ is given by Eq. (23).

It is of interest to compare $W_C(\tau)$ in the constant flux approximation with the time-centered differencing of Eq. (43) which is sometimes argued as "more than adequate." The time-centered representation of Eq. (43) is

$$\underline{E}(t) - \underline{E}(t_0) = \tau \dot{\underline{E}}(\tau/2), \quad (49)$$

where

$$\tau \dot{\underline{E}}(\tau/2) = F W_D(\tau/2) A^{-1} \underline{M}(t). \quad (50)$$

$$W_D(\tau/2) = \tau (I + S_0 \tau/2). \quad (51)$$

This result is just $W_C(\tau/2)$ terminated after the second term in $D(C)$, since from Eq. (23)

$$D(C) = C^{-1}(e^C - I) \approx I + \frac{C}{2} + \frac{C^2}{3!} + \dots \quad (52)$$

Thus $W_D(\tau/2)$ will give a correct result only provided $\frac{|| (S_0 \tau)^2 ||}{4!} \ll 1$, where $S_0 \propto \theta \sigma$.

It is usually the case in energy production problems that there is some dominant time interval τ_d determined from the constant flux approximation time interval, τ_c , and from other physical processes, τ_p , of the modeling under consideration. Then

$$\tau_d = \min (\tau_c, \tau_p). \quad (53)$$

If $\alpha_d = ||S_0 \tau_d|| > 10^{-2}$ and $M > 2$ accuracy is required (see Table I), then using the time-centered differencing given by Eq. (51) with result in computation times a factor R slower than the matrix operator methods, Eq. (48), where R is given in Table II.

On the other hand, if $\tau_p \ll \tau_c$, we have a problem that is strongly driven by τ_p . If, in addition, $||S_0 \tau_p|| < 10^{-2}$ and $M \approx 2$ accuracy is adequate, then the time-centered differencing could prove to be adequate. However, if at some stage of the problem evolution the above special conditions were reversed, i.e., $||S_0 \tau|| > 10^{-2}$, then the resulting increase in computer time could be significant if not catastrophic. Of course if these criteria occur and are ignored by the calculation, negative densities result (unless set to zero), which is impossible. The matrix operator method automatically adjusts to these limiting conditions, and is preferred in all instances.

In the special case of pure decay problems resulting in lower triangular matrices, the largest diagonal element λ will determine the maximum time step allowed by time-centered differencing as

$$\lambda \tau \ll 1. \quad (54)$$

In typical applications for reactors this restriction is too severe to adequately perform the calculation. Analytic solutions for more than about three or four isotopes in a branching chain are quite complicated. For ten isotopes the problem is practically unmanageable if solved analytically for arbitrary radioactive chains.

The problem of evaluating $W(\tau)$ given by Eq. (47) for the linear flux approximation, $S = S_0 (a + b\tau)$, and the exponential flux approximation, $S = S_0 e^{\alpha\tau}$, where a , b , and α are scalars, has also been investigated. Although one may readily demonstrate a symbolic representation in terms of exponentials, error functions or exponential integrals, we have not yet determined a complete computational scheme valid for all $||S_0 \tau||$. This problem is under investigation.

ACKNOWLEDGMENTS

The author wishes to express his gratitude to the Aspen Center for Physics, the National Science Foundation, and the Energy Research and Development Administration under whose auspices this research was performed.

REFERENCES

1. F. F. Gantmacher, The Theory of Matrices (Chelsa Publishing Company, New York, 1960) Vol II, pp. 125ff, 185ff.
2. G. I. Bell and S. Glasstone, Nuclear Reactor Theory (Van-Nostrand Reinhold Company, New York, 1970), pp. 562 ff.
3. E. Bodewig, Matrix Calculus (Interscience Publishers, New York, 1963) pp. 67ff.
4. H. B. Duane, "Transmutation Logic For S_n Transport Analysis," Proc. Conf. Appl. of Computing Methods to Reactor Problems, Argonne National Laboratory report ANL-7050 (1965).