12

THE THEORY FOR THE NUMERICAL SOLUTION OF TIME-DEPENDENT AND TIME-INDEPENDENT MULTI-GROUP DIFFUSION EQUATIONS

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The Theory for the Numerical Solution of Time-Dependent and Time-Independent Multigroup Diffusion Equations*

By R. S. Varga† and M. A. Martino‡

1. Introduction

It has long been recognized that the multigroup diffusion theory approximations to the transport equation give very useful information in the nuclear design of many types of reactors. In recent years, the solutions of these multigroup diffusion equations have been attacked numerically by means of large-scale digital computers.§ In this paper, mathematically rigorous foundations are given for the time-dependent and time-independent multigroup approximations, not only for the discrete (space) numerical problem consisting of a finite number of mesh (lattice) points, but for the continuous space problem as well. In so doing, the discrete numerical approximations to the multigroup diffusion equations, as solved on digital machines, will be shown to be well-set.

2. Statement of the Problems

Let the domain of the reactor R be a finite connected region in n-dimensional Euclidean space, $n \leq 3$, with R equal to the union of a finite number of disjoint convex sub-regions‖ $R_1, R_2, \ldots, R_l$. Let Γ denote the exterior boundary of R, and let γ denote the internal boundaries of R.¶ If the number of lethargy groups is m, then (Ref. 2, p. 291) the time dependent multigroup diffusion equations are:

$$\left[\frac{\partial\phi_i(x,t)}{\partial t} = v_i\left\{\operatorname{div}\,(D_i(x)\,.\operatorname{grad}\phi_i(x,t)) - \sigma_i(x)\phi_i(x,t)\right.\right.$$

$$\left.\left. + \sum_{j\neq i}\sigma_{i,j}{}^{(r)}(x)\phi_j(x,t)\right\}\right]_{i=1}^{m}, \quad x\in R_k, \quad 1\leq k\leq l \qquad (1)$$

where

$$\sigma_i(x) \equiv \sigma_i{}^{(a)}(x) + \sum_j \sigma_{j,i}{}^{(r)}(x). \qquad (2)$$

The quantity $\phi_i(x, t)$ is the neutron flux in the ith lethargy group, and v_i is the average velocity of the neutrons in this group; $D_i(x)$ is the diffusion coefficient, $\sigma_i(x)$ is the total cross-section, and $\sigma_{i,j}{}^{(r)}(x)$ is the slowing-down cross-section from the jth to the ith lethargy group. We have assumed that these latter quantities are time-independent, so that changes in these quantities due to depletion, poisoning, expansion by fission heating, etc., are ignored. By virtue of their physical definitions, we have, for $1 \leq i, j \leq m$,

$$\left.\begin{array}{l} 1.\ D_i(x) \geq \delta > 0 \text{ for all } x\in R \\ 2.\ \sigma_i(x) \geq 0 \text{ for all } x\in R \\ 3.\ \sigma_{i,j}{}^{(r)}(x) \geq 0 \text{ for all } x\in R. \end{array}\right\} \qquad (3)$$

We further assume, for $1 \leq i \leq m$, that

$$\left.\begin{array}{l} 1.\ \phi_i(x,t) \text{ is continuous in } x,\ x\in R, \text{ for all } t\geq 0 \\ 2.\ D_i(x)\dfrac{\partial\phi_i(x,t)}{\partial n} \text{ is continuous across any in-} \\ \quad \text{ternal boundary, } x\in\gamma, \text{ for all } t\geq 0. \end{array}\right\} \qquad (4)$$

On Γ, the external boundary of R, we assume for simplicity the extrapolated (homogeneous) boundary condition** (Ref. 2, p. 103):

$$\phi_i(x,t) + \alpha_i(x)\frac{\partial\phi_i(x,t)}{\partial n} = 0, \quad x\in\Gamma, \qquad (5)$$

where $\alpha_i(x)$ is continuous and non-negative on Γ.

For the time-independent multigroup diffusion problem, we have, for $x\in R_k$,

$$\left\{-\operatorname{div}(D_i(x)\,.\operatorname{grad}\phi_i(x)) + \sigma_i(x)\phi_i(x)\right.$$

$$\left. = \sum_{j<i}\sigma_{i,j}{}^{(r)}(x)\phi_j(x) + \frac{\chi_i\psi(x)}{\lambda}\right\}_{i=1}^{m}, \qquad (6)$$

* The theoretical work for Sections 3–5 is due jointly to Professor Garrett Birkhoff of Harvard University and the first author. The theoretical work for Sections 6–10 is due jointly to Dr. G. J. Habetler‡ and the second author.

† Bettis Atomic Power Division, operated for the U.S. Atomic Energy Commission by the Westinghouse Electric Corporation.

‡ Knolls Atomic Power Laboratory, operated for the U.S. Atomic Energy Commission by the General Electric Company.

§ See Ref. 1 for the range of existing machine codes currently being used in the design of water-moderated reactors.

‖ The assumptions here concerning the domain R of the reactor are, for reasons of brevity, overly restrictive. For example (Ref. 8), the results for the discrete problem hold for arbitrary dimension n. See also Ref. 20.

¶ Precisely, $\gamma = \bigcup_{i=1}\{\bar{R}_i - R_i\} - \Gamma$, where $\bar{R}_i$ denotes the closure of R_i.

** The normal derivative here refers to the outward normal.

where the fission source of neutrons, $\psi(x)$, is defined by:

$$\psi(x) = \sum_i [\nu\sigma_f(x)]_i \phi_i(x). \tag{7}$$

The probabilities χ_i are non-negative scalars with $\sum_i \chi_i = 1$. The quantity $[\nu\sigma_f(x)]_i$ is related to the macroscopic fission cross section, and is thus non-negative. The homogeneous boundary conditions of (5), and the continuity conditions of (4), are also assumed to apply, in the time-independent problem, to the fluxes $\phi_i(x)$, as well as to the fission source $\psi(x)$.

For the time-dependent problem, we seek solutions of (1) for given initial conditions, and we are especially interested in the behavior of $\phi_i(x, t)$ for large positive values of t. For the time-independent problem, which is an eigenvalue problem, we seek to determine solutions of (6) corresponding to the largest (in modulus) eigenvalue λ of (6).

The theoretical results, and the methods for proving these results for the discrete and continuous space problems, are interesting in their own light, and will be treated separately. The basic tools used in proving the results in these different sections are, however, quite similar. The Perron-Frobenius theory (Refs. 7, 9, 10) of non-negative square matrices (which obviously leave the positive hyperoctant invariant) is the basis for results for the discrete space problems, whereas the abstraction of the Perron-Frobenius theory by Krein and Rutman (Ref. 17) to linear operators which leave a cone invariant in a Banach space is the basis for the results for the continuous space problems.

DISCRETE SPACE

3. Derivation of the Difference Equations and Properties of the Derived Matrices

For simplicity in exhibition, we now assume that the dimension of the space is $n = 2$, and that the subregions R_i are rectangles. This enables us to impose a mesh Λ of horizontal and vertical line segments on the plane in such a way that all interfaces between subregions, and all external boundaries coincide with segments of Λ. The mesh spacings in the x and y directions need not be constant. With the mesh Λ, the unknowns, numbering N, for the ith lethargy group in the discrete case are then defined to be the values of ϕ_i at the intersections of the horizontal and vertical lines of Λ. By replacing the differential equations of (1) and (6) with difference equations in the unknowns of the discrete case, we define the discrete time-dependent and discrete time-independent problems.

On the mesh Λ, the differential operator (in Cartesian coordinates), $-\text{div}\,[D_i(x)\,\text{grad}] + \sigma_i(x)$, is replaced†† explicitly (Ref. 3, pp. 53–54) with an $N \times N$ matrix A_i. We now make the following

DEFINITION 1. A square matrix $M = \| m_{i,j} \|$ is *irreducible*‡‡ if, for any i and j, there exists a finite sequence of integers $k(0) = i, k(1), \ldots, k(r) = j$, such that $m_{k(h-1),k(h)} \neq 0$ for $h = 1, 2, \ldots, r$.

THEOREM 1. The $N \times N$ matrix $A_k = \| a_{i,j}^{(k)} \|$ has the following properties:

1. $a_{i,i}^{(k)} > 0$, $a_{i,j}^{(k)} \leqslant 0$ for $i \neq j$, and $a_{i,j}^{(k)} = a_{j,i}^{(k)}$ for $1 \leqslant i, j \leqslant N$, $1 \leqslant k \leqslant m$.
2. $a_{i,i}^{(k)} \geqslant \sum_{j \neq i} |a_{i,j}^{(k)}|$ for all $1 \leqslant i \leqslant N$, with strict inequality for some i.
3. A_k is irreducible.

Thus, each A_k is symmetric and positive definite, and A_k^{-1} is a positive matrix, i.e., each entry of A_k^{-1} is strictly positive.

PROOF. The first statement follows by construction (Ref. 3), utilizing the inequalities of (3). The boundary conditions (5), coupled with the connectivity of the reactor R, give the diagonal dominance of the matrices A_k, as well as their irreducibility. Matrices satisfying statements 2 and 3 have non-vanishing determinants (Ref. 4), and it follows that if λ is any negative real number, then $A_k - \lambda I$ is also diagonally dominant, and hence has a non-zero determinant. Evidently, A_k is then positive definite. The conclusion concerning A_k^{-1} is an extension (Refs. 5, 6) of an old result due to Stieltjes.

Further properties of the derived matrices A_k are numerically important. For example (Ref. 2), it can be shown that the matrices A_k satisfy Young's *property* (A) (Ref. 12), and that the Young-Frankel (Ref. 12, 13) *successive overrelaxation method* can be rigorously applied to matrix equations of the form:

$$A_k \mathbf{x} = \mathbf{k}. \tag{8}$$

If $\boldsymbol{\phi}_i$ represents a column vector with N components, then returning to problems (1) and (6), we have as their discrete matrix analogues:

$$\left\{ \frac{\partial \boldsymbol{\phi}_i}{\partial t} = v_i \left(-A_i \boldsymbol{\phi}_i + \sum_{j \neq i} B_{i,j} \boldsymbol{\phi}_j \right) \right\}_{i=1}^{m} \tag{9}$$

and

$$\left\{ A_i \boldsymbol{\phi}_i = \sum_{j<i} B_{i,j} \boldsymbol{\phi}_j + \frac{\chi_i \boldsymbol{\psi}}{\lambda} \right\}_{i=1}^{m}, \tag{10}$$

where

$$\boldsymbol{\psi} = \sum_i V_i \boldsymbol{\phi}_i. \tag{11}$$

The quantities $B_{i,j}$ and V_i are (Ref. 3), by virtue of derivation, diagonal matrices. Moreover, from (3), they are non-negative diagonal matrices.

4. The Discrete Time-Independent Problem

We shall first transform our matrix equations (10), (11) into a more compact form. From (10), we have:

†† The method described in Ref. 3 permits of an easy extension to higher dimensions. The results of Theorem 1 apply to higher dimensional cases as well.

‡‡ This is also called *indecomposable*, and transitive. See Refs. 9, 10, 11.

$\phi_1 = \chi_1 A_1^{-1}(\psi/\lambda)$; $\phi_2 = A_2^{-1}\{\chi_1 B_{2,1} A_1^{-1} + \chi_2 \cdot I\}(\psi/\lambda)$, and, in general,

$$\phi_i = L_i(\psi/\lambda), \quad 1 \leqslant i \leqslant m. \tag{12}$$

If we define $T \equiv \sum_i V_i L_i$, then, from (11), we obtain

$$T\psi = \lambda\psi. \tag{13}$$

We may assume, without loss of generality, that $\chi_1 > 0$. Since the entries of the non-negative diagonal $B_{i,j}$, $j < i$, arise from slowing down cross sections, we are led by the physics to assume that at least $B_{i,i-1}$, $1 < i \leqslant m$, is a positive diagonal matrix. Thus, since A_i^{-1} is a positive matrix from Theorem 1, we can inductively show that each L_i, $1 \leqslant i \leqslant m$, is also a positive matrix. By definition, each matrix V_i is a non-negative diagonal matrix. We now assume that at least one of the sub-regions R_k contains some fissionable material. By the same permutation of rows and columns of the matrices V_i, we have:

$$V_i = \begin{bmatrix} d_1(i) & & & 0 \\ & d_2(i) & & \\ & & \ddots & \\ 0 & & & d_N(i) \end{bmatrix}, \tag{14}$$

and there exists a non-negative integer r such that $d_l(i) = 0$ for $1 \leqslant i \leqslant r$, for all $1 \leqslant l \leqslant m$, and for at least one l, say l^*, $d_{l^*}(i) > 0$ for $r+1 \leqslant i \leqslant N$. From the definition of T, we then have

$$T = \left[\begin{array}{c|c} 0 & 0 \\ \hline T_1 & T_2 \end{array}\right], \tag{15}$$

where T_1 is an $(N-r)\times r$ matrix, and T_2 is a square $(N-r)\times(N-r)$ matrix. It thus follows that T_2 is a positive matrix, using the fact that each L_i is a positive matrix. Now, the eigenvalues of T are the $(N-r)$ eigenvalues of T_2 and an r-fold zero eigenvalue. By a theorem of Perron (Ref. 7), T_2 possesses an eigenvalue λ^* which is positive, simple, and greater in modulus than all other eigenvalues of T_2. Moreover, to λ^* can be associated a unique§§ eigenvector ψ^* of T_2 with positive components. This is the basis of our

THEOREM 2. The largest (in modulus) eigenvalue λ^* of T is positive, simple, and its corresponding unique eigenvector Ψ can be chosen to have non-negative components. Furthermore, for any arbitrary positive vector ψ_0, the iteration procedure:

$$T\psi_n = \mathbf{S}_{n+1};\quad \lambda_{n+1} = \frac{(\mathbf{S}_{n+1}, \psi_n)}{(\psi_n, \psi_n)};$$
$$\psi_{n+1} = \mathbf{S}_{n+1}/\lambda_{n+1}, \quad n \geqslant 0 \tag{16}$$

is convergent, and

$$\lim_{n\to\infty} \psi_n = c\Psi, \qquad \lim_{n\to\infty} \lambda_n = \lambda^*, \tag{17}$$

where c is some positive scalar.

PROOF. The first assertion is a direct consequence of Perron's theorem (Ref. 7). The convergence of the iteration procedure is guaranteed by the fact that λ^* exceeds in modulus all other eigenvalues of T.

COROLLARY. If

$$\bar{\lambda}_{n+1} = \max_i \left(\frac{S_{n+1,i}}{\psi_{n,i}}\right) \text{ and } \underline{\lambda}_{n+1} = \min_i \left(\frac{S_{n+1,i}}{\psi_{n,i}}\right),$$

where $S_{n+1,i}$ denotes the ith component of $\mathbf{S}_{n+1}$, and the subscript i varies over the range of T, then

$$\underline{\lambda}_{n+1} \leqslant \underline{\lambda}_{n+2} \leqslant \bar{\lambda}_{n+2} \leqslant \bar{\lambda}_{n+1}, \qquad n \geqslant 0 \tag{18}$$

and

$$\underline{\lambda}_{n+1} \leqslant \lambda^* \leqslant \bar{\lambda}_{n+1}, \qquad n \geqslant 0. \tag{19}$$

PROOF. That $\underline{\lambda}_{n+1} \leqslant \lambda^* \leqslant \bar{\lambda}_{n+1}$ follows from a result by Collatz‖‖ (Ref. 14). The nested property of (18) follows easily from the fact that T_2 is a positive matrix.

We remark that Theorem 2 gives the well-set nature of the discrete time-independent eigenvalue problems. Thus, machine computations based on (16) are convergent. Equation (19) of the Corollary gives for each iteration non-trivial upper and lower bounds on λ^*, which is of considerable practical use, since λ^* corresponds physically to k_{eff}.

5. The Discrete Time-Dependent Problem

If $\mathbf{N}(t)$ is a vector with $m.N$ components¶¶ $\frac{1}{v_1}\phi_1(t), \ldots, \frac{1}{v_m}\phi_m(t)$, then Eq. (9) can be written as:

$$\frac{d\mathbf{N}(t)}{dt} = Q\mathbf{N}(t), \tag{20}$$

where the entries of Q are determined*** from the entries of the matrices A_1 and $B_{i,j}$. From Theorem 1, it follows that the matrix $Q = \|q_{i,j}\|$ is such that:

$$q_{i,i} < 0,\ q_{i,j} \geqslant 0 \quad \text{for } i \neq j,\ 1 \leqslant i, j \leqslant m.N. \tag{21}$$

We shall call such matrices *essentially non-negative matrices*. It is known (Ref. 8) that any essentially non-negative matrix has a non-negative eigenvector. We now define a matrix Q to be *essentially positive* if, and only if, it is essentially non-negative and irreducible. Thus, if we assume, as before, that each matrix $B_{i,i-1}$ $1 < i < m$ is a positive diagonal matrix, and that some diagonal element of $B_{m,1}$ is positive, then the matrix Q of (20) is essentially positive. This fact depends on the irreducible nature of the matrices A_i, following from Theorem 1. We have (Ref. 8; p. 10)

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§§ Up to scalar factors.

‖‖ For expressions of the min-max nature of λ^*, see Ref. 3, p. 58, and Ref. 8, p. 28.

¶¶ Thus, $\mathbf{N}(t)$ is related to the total neutron density in the reactor. See Ref. 2, p. 47.

*** The velocity factors v_i have been absorbed into the entries of the matrix.

THEOREM 3. The (essentially positive) matrix Q has a unique strictly positive eigenvector $\mathbf{\Phi}$, with real, and simple, eigenvalue $\mu_1 = M$. Moreover, $\mu_1 > \mathrm{Re}\{\mu_j\}$ for any other eigenvalue μ_j of Q.

Obviously, (off-diagonal) non-negativity and irreducibility are unaffected when a matrix Q is replaced by its transpose Q'. Hence, the transpose Q' of an essentially positive matrix Q is also essentially positive, so that we can apply Theorem 3 to Q'. The positive eigenvector $\mathbf{F}$ of Q' is called the *importance vector* of Q, and its corresponding eigenvalue is $\mu_1 = M$, since Q and Q' have the same characteristic polynomial. We have (Ref. 8, p. 16)

THEOREM 4. For any essentially positive matrix Q, if $\mathbf{N}(0)$ is a positive vector, then

$$\mathbf{N}(t) = Ke^{Mt}\mathbf{\Phi} + o(e^{\mu t}), \quad t \to \infty, \tag{22}$$

where $\mathbf{\Phi}$ and M are as in Theorem 3, μ is some number strictly between M and $\sup_{j>1} \mathrm{Re}\{\mu_j\}$, and $K = (\mathbf{F}, \mathbf{N}(0))/(\mathbf{F}, \mathbf{\Phi})$, $\mathbf{F}$ being the importance vector of Q.

Thus, we have obtained, in the discrete time-dependent case, the asymptotic behavior of $\mathbf{N}(t)$ for t large. This leads us naturally to

DEFINITION 2. For Q essentially positive, the process (20) will be called *subcritical*, *critical*, or *supercritical*, according as $M < 0$, $M = 0$, or $M > 0$ in Theorem 4.

COROLLARY. Let Q be any essentially positive matrix. For $\mathbf{N}(0)$ a positive vector, if we define $\|\mathbf{N}(t)\| = \sum_i N_i(t)$, so that $\|\mathbf{N}(t)\|$ is the (expected) total number of neutrons at time t, then

$$\lim_{t\to\infty} \|\mathbf{N}(t)\| = \begin{cases} +\infty, \text{ if the process is supercritical,} \\ \text{finite, if the process is critical,} \\ 0, \text{ if the process is subcritical.} \end{cases} \tag{23}$$

CONTINUOUS SPACE

6. Definition and Properties of the Operators

In the analysis to follow, we shall assume that the quantities $D_i(x)$, $\sigma_i(x)$, and $\sigma_{i,j}^{(r)}(x)$ have continuous and bounded second-order partial derivatives in the interior of each sub-region R_i, $1 \leqslant i \leqslant l$. Let $\Phi(x) \equiv (\phi_1(x), \phi_2(x), \ldots, \phi_m(x))$, where $\phi_j(x)$ has bounded second-order derivatives in the interior of each sub-region R_i. A function $\Phi(x)$, satisfying these assumptions, as well as the boundary conditions of (4) and (5), will be said to belong to class C, denoted $\Phi \in C$.

We now define two operators, $\mathscr{D}$ and α:

$\Phi(x) \equiv (\omega_1(x), \ldots, \omega_m(x))$, with

$$\omega_j(x) = \theta_j\phi_j(x) = \mathrm{div}\,[D_j(x)\,\mathrm{grad}\,\phi_j(x)],$$

$\Phi(x) \equiv (Z_1(x), \ldots, Z_m(x))$, with

$$Z_i(x) = -\sigma_i(x)\phi_i(x) + \sum_{j\neq i} \sigma_{i,j}^{(r)}(x)\phi_j(x).$$

The multigroup diffusion operator Q, defined on C, is:

$$Q\Phi = \mathscr{D}\Phi + \alpha\Phi, \tag{24}$$

and the time-dependent (kinetics) multigroup diffusion equations become:†††

$$\frac{\partial\Phi(x,t)}{\partial t} = Q\Phi(x,t), \tag{25}$$

where $\Phi(x, t) \in C$ for each fixed $t \geqslant 0$.

Concerning (25), two questions immediately arise. First, for a given initial function $\Phi(x, 0)$ satisfying reasonable continuity conditions, does there exist a solution of (25)? Second, if so, what is its asymptotic behavior for large values of t?‡‡‡

By means of modern spectral theory for unbounded self-adjoint operators on a Banach space, a complete answer to these questions will be given for the general one-dimensional multigroup model and for arbitrary dimension in the case of the homogeneous reactor. A less complete theory covering special $\Phi(r, 0)$ will be shown for the general three-dimensional case. The principal tool in this analysis is an extension of Jentzsch's theorem[15, 16] on integral operators with positive kernels, obtained by M. G. Krein and M. A. Rutman (Ref. 17) in their study of operators leaving invariant a cone in a Banach space. The result used here is:

THEOREM 5. Suppose the non-negative kernel $K(s, t)$ satisfies $\iint_{R\times R} |K(s,t)|^2\, dV_s dV_t < +\infty$, and that $K(s, t) > 0$ except possibly on a set of measure zero. Then, the integral equation:

$$\int_R K(s,t)\phi(t)\, dV_t = \lambda\phi(s) \tag{26}$$

has a single non-negative solution, positive almost everywhere, for some positive number λ which exceeds the modulus of all other eigenvalues of (26). For the same value of λ the adjoint equation:

$$\int_R K(t,s)\psi(t)\, dV_t = \lambda\psi(s)$$

has a solution $\psi(s)$ which is positive almost everywhere.

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††† Problems involving the addition of an extraneous source S:

$$\frac{\partial\Phi}{\partial t} = Q\Phi + S$$

are also treated in Refs. 8 and 20.

‡‡‡ A naïve answer to the first question might be

$$\Phi(x,t) = e^{tQ}\Phi(x,0) = \sum_{k=0}^{\infty} \frac{t^k Q^k}{k!}\Phi(x,0). \tag{38}$$

Indeed, if $\Phi(x, 0)$ and the coefficients of $\mathscr{D}$ and α are sufficiently regular, Eq. (38) will be a valid solution of (25). However, for a heterogeneous reactor model, the coefficients of Q are generally discontinuous across material interfaces γ so that the terms of the series (38) do not satisfy the admissibility conditions for C, and are lacking for physical interpretation. Even in those special cases where (38) is valid, this form of the solution does not offer a direct insight into the second question.

The analysis of Q is carried out by imbedding the class C in the Hilbert space H of complex-valued functions $\Phi=(\phi_1, \phi_2, \ldots, \phi_n)$ defined on R almost everywhere and for which $\|\Phi\|=\sum_{j=1}^{n}\int_R |\phi_j(x)|^2\, dV_x$ is finite. Each of the differential operators θ_j is self-adjoint on C and possesses a Green's function $G_j(x, y)$. The operator $\mathscr{D}^{-1}$ defined on H by:

$$\mathscr{D}^{-1}\Phi(x)=\left(\int_R G_1(x, y)\phi_1(y)\, dV_y, \ldots, \int_R G_m(x, y)\phi_m(y)\, dV_y\right)$$

is inverse to $\mathscr{D}$ in the sense that $\mathscr{D}^{-1}\mathscr{D}\Phi=\Phi$ for all $\Phi\in C$. Since $\mathscr{D}^{-1}$ is defined everywhere on H, $\mathscr{D}$ can be extended to the range R of $\mathscr{D}^{-1}$ by setting $\mathscr{D}(\mathscr{D}^{-1}\Phi)=\Phi$ for all $\Phi\in H$; we assume $\mathscr{D}$ is so extended.

$\mathscr{D}^{-1}$ is self-adjoint and completely continuous (i.e., it maps every bounded set into a compact set) on H. Hence (Ref. 18) $\mathscr{D}^{-1}$ possesses a complete orthonormal sequence of eigenfunctions $\{\Omega_j(x)\}$ where $\mathscr{D}^{-1}\Omega_j=(1/\omega_j)\Omega_j$, with $\omega_j<0$ for $j=1, 2, \ldots$. The negativity of the eigenvalues of $\mathscr{D}^{-1}$ follows from the negativity of the eigenvalues of each θ_k^{-1}, $1\leqslant k\leqslant m$, which in turn is obtained from Green's Theorem as follows. Assume $\theta_k\phi=\lambda\phi$. Since θ_k is self-adjoint, $\phi(x)$ can be assumed to be real valued. Thus,

$$\lambda\int_R \phi^2(x)\, dV_x=\int_R \phi(x)\theta_k\phi(x)\, dV_x$$
$$=-\int_R D_k(x)\,\|\operatorname{grad}\phi\|^2\, dV_x + \int_\Gamma D_k(x)\phi\frac{\partial\phi}{\partial n}\, d\sigma. \quad (27)$$

The positive nature of the D_k and the boundary condition (5) show that the terms of the right member of (27) are non-positive, vanishing only if $\phi\equiv$ constant. In the latter case, the boundary condition (5) implies that $\phi\equiv 0$, contradicting the assumption that ϕ is an eigenfunction. Thus, $\lambda<0$.

7. The Homogeneous Reactor

In the case of the single region reactor with constant coefficients D_i, $\sigma_{i,j}^{(r)}$, σ_i, with group-independent boundary conditions (i.e., $a_i(r)$ in (5) is independent of i) the theory is particularly simple, and will be given first.

THEOREM 6. For the homogeneous model, Q has a complete sequence of generalized eigenfunctions (Ref. 24, pp. 67–70):

$$\begin{array}{lll} \Phi_0= & \Phi_{0,0} & \\ \Phi_{1,0}, & \Phi_{1,1}, \ldots, & \Phi_{1,k_1} \\ \vdots & \vdots & \vdots \\ \Phi_{j,0}, & \Phi_{j,1}, \ldots, & \Phi_{j,k_j} \\ \vdots & \vdots & \vdots \end{array}$$

corresponding to eigenvalues $\lambda_0, \lambda_1, \lambda_2 \ldots$. That is,

$$Q\Phi_{i,0}=\lambda_i\Phi_{i,0},$$
$$Q\Phi_{i,j}=\lambda_i\Phi_{i,j}+\Phi_{i,j-1}, \quad 1\leqslant j\leqslant k_i, \quad i=1, 2, \ldots$$

There exists an eigenvalue, λ_0, which is real, simple, and algebraically larger than the real part of all other eigenvalues: $\lambda_0>\sup_{j>1}\operatorname{Re}\{\lambda_j\}$. The adjoint equations:

$$Q^*\Psi_{i,0}=\bar{\lambda}_i\Psi_{i,0},$$
$$Q^*\Psi_{i,j}=\bar{\lambda}_i\Psi_{i,j}+\Psi_{i,j-1}, \quad 1\leqslant j\leqslant k_i,\ i=1, 2, \ldots$$

have solutions. Φ_0 and $\Psi_0=\Psi_{0,0}$ are positive in the interior of R and all the $\Phi_{i,j}$ and $\Psi_{i,j}$ belong to class C. Every function $\Phi\in H$ has a conditionally convergent bi-orthogonal expansion

$$\Phi=\sum_{i,j}(\Phi, \Psi_{i,k_i-j})\Phi_{i,j}.$$

The solution to Eq. (25) for

$$\Phi(x, 0)=\sum_{i,j} a_{ij}\Phi_{i,j}(x)\in C$$

is:

$$\Phi(x, t)=e^{tQ}\,\Phi(x, 0)=\sum_{i,j} a_{i,j}\, e^{\lambda_i t}\sum_{q=0}^{j}\frac{\Phi_{i,q}(x)}{(j-q)!}t^{(j-q)}. \quad (28)$$

If $\Phi(x, 0)\geqslant 0$ and $\Phi(x, 0)\not\equiv 0$ then $a_{0,0}>0$ and $\Phi(x, t)$ is asymptotic to $a_{0,0}\, e^{\lambda_0 t}\Phi_0$ for large t.

PROOF. Let $l_0(x)$, $l_1(x)$, ... be a complete orthonormal set of eigenfunctions for the Laplacian operator, satisfying the boundary conditions

$$l_k(x)+a(x)\frac{\partial l_k}{\partial n}=0 \text{ on } \Gamma.$$

Thus,

$$\nabla^2 l_k(x)=\mu_k l_k(x), \quad x\in R.$$

Define $\mathscr{M}_k$ to be the subspace of H consisting of all functions Φ of the form $\Phi=(a_1 l_k, a_2 l_k, \ldots, a_m l_k)$, where the a_j are arbitrary complex numbers. Each $\mathscr{M}_k$ is an m-dimensional subspace of H, invariant under Q. Thus, the Jordan canonical form of any matrix representation of Q restricted to $\mathscr{M}_k$ shows that $\mathscr{M}_k$ is spanned by m generalized eigenvectors of Q, say $\eta_j^{(k)}=(\eta_{j,1}l_k, \ldots, \eta_{j,m}l_k)$, $1\leqslant j\leqslant m$. Hence, every $\Phi\in H$ has an expansion $\Phi=\sum_k c_k\Lambda_k$, where $c_k\Lambda_k$ is the projection of Φ on $\mathscr{M}_k$, given by the usual bi-orthogonal expansion in $\mathscr{M}_k$. Since the Λ_k are orthogonal, the expansion for Φ converges absolutely. However, each $c_k\Lambda_k$ is in turn expressible as a sum $\sum_{j=1}^{m} b_{j,k}\eta_j^{(k)}$ and the double series:

$$\Phi=\sum_{j,k} b_{j,k}\eta_j^{(k)}$$

need not be absolutely convergent. The necessity for the proper grouping of terms in the bi-orthogonal expansions is accented in the general model.

The Laplacian operator, ∇^2, with the given boundary conditions, has an inverse, ∇^{-2}, which is an integral operator with negative kernel. So, $-\nabla^{-2}$ satisfies the conditions of Theorem 5. As far as real negative eigenvalues of ∇^2 are concerned, ∇^2 possesses a unique largest, simple eigenvalue μ_0 corresponding to an eigenfunction, say l_0, which is positive in the interior of R. The eigenvalues of Q consist of the set of eigenvalues of the matrices:

$$M_k = \mu_k D + \mathfrak{a}$$

where D is the (positive) diagonal matrix of (constant) diffusion coefficients, and $\mathfrak{a}$ is as before. Each M_k is *essentially positive* (in the sense of Section 5), and hence possesses a positive eigenvector $v_k = (v_{k,1}, v_{k,2}, \ldots, v_{k,m})$ corresponding to a real, simple eigenvalue ρ_k with maximal real part. If $\rho_0 > \rho_k$, $k > 0$, then clearly $\Phi_0 = v_0 \cdot \Lambda_0$ and $\lambda_0 = \rho_0$ satisfy the statements of Theorem 6. To show the dominance of $\rho_0 = \lambda_0$, let $w_k = (w_{k,1}, \ldots, w_{k,m})$ be the positive eigenvector for the adjoint equation $M_k^* w_k = \rho_k w_k$. It easily follows that $\rho_0 - \rho_k = \frac{(\mu_0 - \mu_k)(v_0, D_{w_k})}{(v_0, w_k)}$, which is positive, since v_0 and w_k are positive vectors.

The validity of (28) and the differentiability claims for the generalized eigenfunctions, as well as other details of this theory, are in Refs. 19 and 20.

8. The General One-Dimensional Model

The supremum norm of an operator U on H will be denoted by $|||U||| = \underset{\Phi \neq 0}{\text{l.u.b.}} \frac{\|U\Phi\|}{\|\Phi\|}$. An operator with finite norm is termed "bounded". Returning to the general multigroup operator $Q = \mathscr{D} + \mathfrak{a}$, it is observed that $\mathfrak{a}$ is bounded. As before, we denote the eigenvalues of $\mathscr{D}$ by $\{\omega_j\}$, and we denote $R_a = (aI - Q)^{-1}$ for any complex number a. R_a is termed the *resolvent* of Q and is a bounded operator provided a is not an eigenvalue of Q.

LEMMA. For any complex number a, let $\delta(a) = \min_{j \geq 1} |a - \omega_j|$. If $\delta(a) \geq 2|||\mathfrak{a}|||$, then $|||R_a||| \leq \frac{2}{\delta(a)}$.

PROOF. Let $\Phi \in H$ and let $\Phi = \Sigma a_i \Lambda_i$ be its expansion in the eigenvectors of $\mathscr{D}$. Then

$$(aI - \mathscr{D})^{-1}\Phi = \sum \frac{a_i}{a - \omega_i}\Phi_i,$$

so

$$\|(aI - \mathscr{D})^{-1}\Phi\|^2 = \sum \frac{|a_i|^2}{|a_i - \omega_i|^2} \leq \frac{1}{\delta^2(a)} \sum |a_i|^2 = \frac{\|\Phi\|^2}{\delta^2(a)},$$

hence

$$|||(aI - \mathscr{D})^{-1}||| \leq \frac{1}{\delta(a)}.$$

By assumption,

$$|||\mathfrak{a}(aI - \mathscr{D})^{-1}||| \leq |||\mathfrak{a}|||\cdot|||(aI - \mathscr{D})^{-1}||| \leq \frac{|||\mathfrak{a}|||}{\delta(a)} \leq \tfrac{1}{2}.$$

The Neumann expansion

$$U(a) = (I - \mathfrak{a}(aI - \mathscr{D})^{-1})^{-1} = \sum_{k=0}^{\infty} (\mathfrak{a}(aI - \mathscr{D})^{-1})^k$$

is therefore valid and

$$|||U(a)||| \leq \sum_{k=0}^{\infty} |||(aI - \mathscr{D})^{-1}|||^k \leq \sum_{k=0}^{\infty} \frac{1}{2^k} = 2.$$

Hence $$|||R_a||| = |||(aI - \mathscr{D})^{-1}U(a)||| \leq \frac{2}{\delta(a)}.$$

We now consider the one-dimensional model. A comparison of the Green's function for

$$0 = \frac{d}{dx}\left(D_j(x)\frac{d}{dx}\right)$$

with that for

$$\left(\max_{x \in R} D_j(x)\right)\frac{d^2}{dx^2},$$

and a straightforward computation of the eigenvalues of the latter, shows the existence of a constant k_0 such that the number of eigenvalues ω_j for which $-\omega_j \leq t$ is no more than $k_0\sqrt{t}$. It follows from the above lemma that there is a sequence of concentric circumferences in the complex plane, $C_1, C_2, \ldots$, whose radii $r_1, r_2, \ldots$, tend to infinity with n and such that:

$$\lim_{n \to \infty} \underset{a \in C_n}{\text{l.u.b.}} |||R_a||| = 0. \tag{29}$$

Now Q, defined on R, is a closed operator (Ref. 21). Also $R_a = (aI - \mathscr{D})^{-1}U(a)$ is completely continuous if $\delta(a) > |||\mathfrak{a}|||$, so a theorem of M. A. Naimark (Refs. 22, 23) shows that the generalized eigenfunctions of Q span H. It also follows that there exist a sequence of disjoint circles $c_1, c_2, \ldots$ in the complex plane such that every eigenvalue of Q is interior to one of the c_j, and every $\Phi \in R$ has an absolutely convergent representation:

$$\Phi = \frac{1}{2\pi i}\sum_{k=1}^{\infty}\int_{C_k} R_a \Phi\, da. \tag{30}$$

The terms of (30) are projections on to the subspaces η_k spanned, respectively, by the eigenfunctions and generalized eigenfunctions corresponding to eigenvalues interior to c_k. Equation (30) can be written in the form of a bi-orthogonal expansion:

$$\Phi = \Sigma(\Phi, \Psi_{i,k_{i-j}})\Phi_{i,j} \tag{31}$$

as in Theorem 6. Here it is necessary to group the terms of (31) arising from a common c_k in order to ensure a convergent representation. Thus (30) is a preferred form of the expansion.

THEOREM 7. The results of Theorem 6 extend to the general reactor in the case of one dimension. An absolutely convergent form of the solution of Eq. (25) is:

$$\Phi(x, t) = \frac{1}{2\pi i}\sum_{k=1}^{\infty}\int_{c_k} e^{at}R_a\Phi(x, 0)\, da. \tag{32}$$

PROOF. The proof of Theorem 7 can now be obtained by expanding Φ in generalized eigenfunctions in (32). The result is of the form:

$$\Phi(x, t) = \int_R K_t(x, s)\Phi(s, 0)\, ds. \tag{33}$$

If $\Phi(s, 0) \geqslant 0$, $\Phi(s, 0) \not\equiv 0$, we have from (24):

$$\frac{\partial \Phi}{\partial t} \geqslant \mathscr{D}\Phi(x, t)$$

for all $t \geqslant 0$. It follows that $\Phi(x, t) \geqslant \Phi(x, t)$ where Φ is the solution to the diffusion equation $\partial\Phi/\partial t = \mathscr{D}\Phi$. Thus $\Phi(x, t) > 0$ for all $t > 0$, x in the interior of R. The kernel K_t of (33) is continuous and therefore positive for almost all x and s in the interior of R. Theorem 5 can now be applied to (33) and Theorem 7 follows from the observation that the eigenvalues of Q and (33) are related through λ and e_t^{λ}, respectively.

9. A General Result for λ_0

For the general multigroup operator in arbitrary dimensions we can establish the existence of the fundamental mode and importance function in the following sense.

THEOREM 8. For general Q there exists a simple, real eigenvalue $\lambda_0 \geqslant \mathrm{Re}\{\lambda_k\}$ for all eigenvalues λ_k of Q. The corresponding eigenfunction and adjoint eigenfunction, Φ_0 and Ψ_0, respectively, are strictly positive in the interior of R and are the only eigenfunctions for Q, Q^*, respectively, which are everywhere non-negative.

PROOF. We have already seen that $R_a = (aI - Q)^{-1}$ is completely continuous for sufficiently large positive a. R_a also has a positivity property. Let

$$\gamma = -\min_{1\leqslant j\leqslant n}\ \mathrm{g.l.b.}_{r\in R}\ \sigma_j(x).$$

Then the matrix elements of $\mathfrak{a}_1 = \mathfrak{a} + \gamma I$ are everywhere non-negative. Setting $a_1 = a + \gamma$,

$$R_a = [(a+\gamma)I - \mathscr{D} - (\mathfrak{a} + \gamma I)]^{-1}$$

$$= (a_1 I - \mathscr{D})^{-1} \sum_{k=0}^{\infty} [\mathfrak{a}_1 (a_1 I - \mathscr{D})^{-1}]^k. \tag{34}$$

Here $(aI - \mathscr{D})^{-1}$ is the integral operator with the Green's kernel for the diffusion-absorption operator $\mathscr{D} - aI$. Since this kernel is positive, the right member of (34) is seen to be a positive integral operator for which Theorem 5 applies. Let $\mu_0(a)$ be the eigenvalue of R_a given by Theorem 5. Then $\lambda_0 = a - \frac{1}{\mu_0(a)}$ is a real, simple eigenvalue of Q. Should there be another eigenvalue, say λ_1, for which $\mathrm{Re}\lambda_1 > \lambda_0$ then, for a sufficiently large positive a we will have:

$$|a - \lambda_1| \leqslant (a - \lambda_0),\ \text{so}\ |\mu_1(a)| = \frac{1}{|a-\lambda_1|} \geqslant \frac{1}{a-\lambda_0} = \mu_0,$$

which contradicts Theorem 5 for R_a. This proves Theorem 8.

10. The Time-Independent Problem

The equations for the time-independent model with no up-scattering§§§ are of the form

$$-(\mathscr{D} + S)\Phi = \frac{1}{\lambda} F\Phi, \tag{35}$$

where $\mathscr{D}$ is as before, and $S = \| S_{i,j}(x) \|$ is a lower triangular matrix, with $S_{i,i}(x) \leqslant 0$, $S_{i,j}(x) \geqslant 0$ for $j < i$, and $S_{i,j}(x) = 0$ for $j > i$. The matrix $F = \| F_{i,j}(x) \|$ is non-negative, and is in general singular for certain values of x.

It is easy to verify that $\mathscr{D} + S$ has an inverse, so that λ is not infinite in (35); thus,

$$-(\mathscr{D} + S)^{-1} F\Phi = \lambda\Phi. \tag{36}$$

Consider the range of F, i.e., the set H_1 of all images $\Phi_1 = F\Phi$. In terms of Φ_1, Eq. (36) becomes:

$$-F(\mathscr{D} + S)^{-1}\Phi_1 = \lambda\Phi_1. \tag{37}$$

The operator $-F(\mathscr{D} + S)^{-1}$ leaves H_1 invariant, and is positive on H_1, in the sense of the Krein-Rutman theory. Hence, we obtain:

THEOREM 9. Equation (37) has a dominant eigenvalue λ_0 which is positive and simple, corresponding to a positive eigenfunction and positive adjoint eigenfunction (in H_1). For the general time-independent eigenvalue problem (35) in arbitrary dimension, $\lambda_0 > |\lambda_k|$ for all eigenvalues $\lambda_k \neq \lambda_0$.

§§§ For extensions to the case of up-scattering in the discrete space problem, see Ref. 8, pp. 38–40, and in the continuous space problem, see Ref. 20.

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