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FIRST-ORDER PERTURBATION THEORY AS USED IN THE MULTIGROUP DIFFUSION CODE EXTERMINATOR-2

Melvin Tobias, T. B. Fowler, and D. R. Vondy

ABSTRACT

This paper discusses the application of first-order perturbation theory in the EXTERMINATOR-2 code. The program can be used to calculate the fractional change in multiplication constant per unit change in a macroscopic material constant or per unit change in a specified nuclide density. The equations used are briefly described. The results of test calculations are presented which compare the predictions of perturbation theory with computed Δk values produced by various input parameter changes.

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I. INTRODUCTION

The EXTERMINATOR-2 code[1] now affords the option of a first-order perturbation theory calculation. (The method of calculation is basically that used in the code EQUIPOISE-3A[2] with extensions and improvements. In particular, the application to diffusion constants is different.) This calculation will provide the user with the fractional change in k per unit change in each of the macroscopic material input constants. In addition, the fractional change in k per unit change in nuclide density may be computed for any nuclides specified. That is, if Z is any material parameter, whether a macroscopic constant such as D, B^2, Σ, or a control rod constant, in any group or region, or a nuclide density, the code can calculate the quantity $\frac{1}{k}\frac{\delta k}{\delta Z}$ in first-order perturbation theory. The succeeding sections describe the theory and equations used in this calculation as well as the results of tests made to compare predicted with calculated increments of multiplication constant.

II. THEORY OF THE FIRST-ORDER PERTURBATION APPROXIMATION

As a result of so-called forward calculation, the EXTERMINATOR code produces a solution to the eigenvalue problem

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[1]T. B. Fowler, M. L. Tobias, and D. R. Vondy, EXTERMINATOR-2: A Fortran IV Code for Solving Multigroup Neutron Diffusion Equations in Two Dimensions, USAEC Report ORNL-4078, Oak Ridge National Laboratory (to be published).

[2]C. W. Nestor, Jr., EQUIPOISE-3A, USAEC Report ORNL-3199 Addendum, Oak Ridge National Laboratory, June 6, 1962.

$$kA\phi_o = M\phi_o \ . \tag{1}$$

The multiplication constant k is the largest eigenvalue of the problem. A is a matrix whose elements are leakage, absorption, and group-to-group removal constants; M is a matrix whose elements are fission source constants. The vector ϕ_o is the solution vector of the problem.

Let us consider the related eigenvalue problem

$$(kA - M)\ \phi_i = \omega_i \phi_i \ , \tag{2}$$

where k is the same value determined in Eq. (1). (Clearly, one of the ϕ_i must be the ϕ_o in Eq. (1) and the corresponding ω_i must be zero.) The adjoint problem is

$$(kA^T - M^T)\ \phi_j^* = \omega_j \phi_j^* \ , \tag{3}$$

where the superscript T denotes transposition and ϕ_j^* is the adjoint flux corresponding to eigenvalue ω_j. The transpose of Eq. (3) is

$$\phi_j^{*T}(kA - M) = \omega_j \phi_j^{*T} \ . \tag{4}$$

If we premultiply Eq. (2) by ϕ_j^{*T} and postmultiply both sides of Eq. (4) by ϕ_i, we obtain the pair of equations

$$\phi_j^{*T}(kA - M)\ \phi_i = \omega_i \phi_j^{*T} \phi_i \ , \tag{5}$$

$$\phi_j^{*T}(kA - M)\ \phi_i = \omega_j \phi_j^{*T} \phi_i \ . \tag{6}$$

Subtracting, we obtain

$$(\omega_i - \omega_j)\ \phi_j^{*T} \phi_i = 0 \ . \tag{7}$$

We see that if $i \neq j$, the adjoint fluxes are orthogonal to the forward fluxes.

If we make a perturbation in A or M or both, what is the change in k which results?

$$(k + \delta k)\ (A + \delta A)\ (\phi_o + \delta\phi) = (M + \delta M)\ (\phi_o + \delta\phi)\ . \tag{8}$$

Multiplying out both sides gives:

$$kA\phi_o + k\delta A\phi_o + \delta kA\phi_o + kA\delta\phi + k\delta A\delta\phi + \delta k\delta A\phi_o + \delta kA\delta\phi + \delta k\delta A\delta\phi$$
$$= M\phi_o + \delta M\phi_o + M\delta\phi + \delta M\delta\phi\ . \tag{9}$$

By definition, $kA\phi_o = M\phi_o$. Let us now neglect products of small quantities so that we have the first-order approximation

$$k\delta A\phi_o + \delta kA\phi_o + kA\delta\phi = \delta M\phi_o + M\delta\phi \tag{10}$$

or, rearranged,

$$\delta kA\phi_o = \frac{\delta k}{k} M\phi_o = (\delta M - k\delta A)\ \phi_o - (kA - M)\ \delta\phi\ . \tag{11}$$

If we premultiply Eq. (11) by ϕ_o^{*T}, where ϕ_o^* is the eigenvector of Eq. (3) with $\omega_o = 0$, we have

$$\frac{\delta k}{k}(\phi_o^{*T}\ M\phi_o) = \phi_o^{*T}(\delta M - k\delta A)\ \phi_o - \phi_o^{*T}(kA - M)\ \delta\phi\ . \tag{12}$$

But

$$\phi_o^{*T}(kA - M) = \left[(kA^T - M^T)\ \phi_o^*\right]^T = 0\ . \tag{13}$$

We have then the first-order perturbation theory approximation to $\delta k/k$ as

$$\frac{\delta k}{k} = \frac{\phi_o^{*T}(\delta M - k\delta A)\ \phi_o}{(\phi_o^{*T}\ M\phi_o)}\ . \tag{14}$$

III. APPLICATION OF PERTURBATION THEORY IN EXTERMINATOR-2

In EXTERMINATOR, the forward calculation is done first, establishing ϕ_o and k. The adjoint flux distribution is computed by inserting the

value of k into the equations, transposing A and M and iterating just as in the forward calculation (except that k is fixed) to find ϕ_o^*. With this information it is possible to compute the fractional change in k per unit change in any parameter Z as follows:

$$\frac{\delta k}{k\delta Z} = \frac{\phi_o^{*T}\left(\frac{\delta M}{\delta Z} - k\,\frac{\delta A}{\delta Z}\right)\,\phi_o}{(\phi_o^{*T}\,M\phi_o)} \,. \tag{15}$$

The quantity Z might be any reactor parameter. In particular, the code outputs $\frac{\delta k}{k\delta Z}$ for Z equal to Σ_A, Σ_R, $\Sigma_R(K\to L)$, DB^2, $\nu\Sigma_f$, CR, D, and B^2 for each group and region. Σ_A, DB^2, $\nu\Sigma_f$, D, and B^2 have their usual definitions. By Σ_R we mean the out-scattering cross section from a group; $\Sigma_R(K\to L)$ is the in-scattering cross section from one group K into another, L. The coefficient calculated for Σ_R does <u>not</u> include any compensation for changes in $\Sigma_R(K\to L)$. Conversely, the coefficients computed for the $\Sigma_R(K\to L)$ do not include compensation by Σ_R. CR is the control rod constant. In the case of DB^2, the change is really in B^2 only and D is not perturbed. In the case of D, the effect of D in DB^2 terms is <u>not</u> included. Note that in Eq. (15) no <u>actual</u> changes are considered – only rates of change of matrix elements with respect to parameters. In addition to this standard output, the user may obtain the coefficient for a particular nuclide density. This is computed by summation using the macroscopic reactivity coefficients which have already been described:

$$\frac{\delta k}{k\delta N} = \Sigma\,\frac{\delta k}{k\delta Z_i}\,\frac{\delta Z_i}{\delta N} \,. \tag{16}$$

The computation of Eq. (15) is enormously simplified in practice by the fact that δM and δA have zero elements except over a region or group being considered. Thus, if Z is a macroscopic non-fission cross section in a particular region, the numerator of Eq. (15) would be

$$-\,k\left[\sum_I\sum_J \phi_o^*(I,J,K)\;\phi_o(I,J,K)\;\Delta V(I,J)\right]_M \,,$$

where the double sum extends over the quadrant elements ΔV covering region M. I is the row number and J is the column number of a point in the mesh; K is the group number. If Z is a macroscopic fission cross section, the numerator would be

$$\sum_{KK} \chi(KK) \left[\sum \sum \phi_o^*(I,J,KK)\ \phi_o(I,J,K)\ \Delta V(I,J) \right]_M .$$

In other words, Eq. (15) is a summation of the derivative of neutron balance items with respect to Z weighted by the adjoint flux at each point. For a D it is the weighted sum of the leakages per unit D; this is the most awkward calculation. (It is to be noted that the perturbation calculation methods used in EXTERMINATOR are, for the most part, similar to those used in a prior code EQUIPOISE-3A; the effects of D perturbations are computed differently, however, as the method used for this purpose in the older code is not satisfactory.)

The EXTERMINATOR code will also calculate the importance-weighted mean neutron lifetime and the effective delayed neutron fraction as defined by Gross and Marable.[3] The reader is referred to their paper for details concerning the derivations of the formulas for these quantities. The formulas used in the code are given in Ref. 1.

A simple numerical illustration of the use of Eq. (15) is given in the Appendix.

IV. COMPARISON OF THE RESULTS OF PERTURBATION THEORY WITH DIRECT COMPUTATION

The following table compares Δk increments predicted by perturbation theory for changes in D values and for particular isotope concentration changes with directly computed Δk values. The latter were obtained by taking the difference in k values computed by two EXTERMINATOR cases, one with and one without the specified changes.

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[3]E. E. Gross and J. H. Marable, Static and Dynamic Multiplication Factors and Their Relation to the Inhour Equation, Nucl. Sci. Eng., 7(4): 281-291 (1960).

The computations were made for reasonably realistic EXTERMINATOR cases, details of which have been omitted for brevity.

Table 1. Comparison of $\Delta k/k$ Values Calculated for Specified Parameter Changes with Those Predicted by Perturbation Theory

A. Diffusion Constant Changes

D	ΔD	$\Delta k/k$, Perturbation Theory	$\Delta k/k$, Direct Calculation
1.52	−0.2	2.0198×10^{-3}	2.1148×10^{-3}
1.32	−0.2	3.3895×10^{-5}	3.66×10^{-5}
1.31	−0.11	8.2408×10^{-6}	8.265×10^{-6}
1.31	−0.2	1.4984×10^{-4}	1.594×10^{-4}

B. Isotope Concentration Changes

ΔN	$\Delta k/k$, Perturbation Theory	$\Delta k/k$, Direct Calculation
-10^{-5}	−0.087387	−0.088605[a]
$+10^{-5}$	+0.087387	+0.086199[a]
-5×10^{-5}	−0.436937	−0.468209
$+10^{-4}$	+0.873875	+0.765291
-10^{-6}	−0.008739	−0.008753[b]
$+10^{-6}$	+0.008739	+0.008726[b]

[a]The average value of $\Delta k/k\ \Delta N$ computed from these two numbers is 8.7402×10^3, to be compared with 8.7387×10^3 calculated from perturbation theory.

[b]The average value of $\Delta k/k\ \Delta N$ computed from these two numbers is 8.7395×10^3.

APPENDIX

SIMPLE NUMERICAL ILLUSTRATION OF THE USE OF EQUATION (15)

Consider a two-group one-dimensional reactor described by four space points; there is a symmetry axis between points 1 and 2 and at

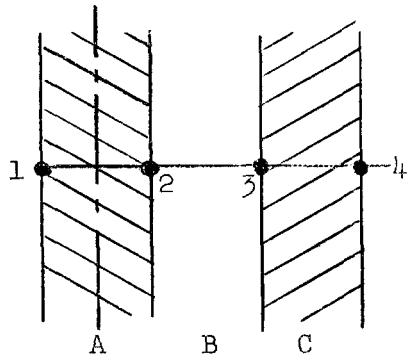

Fig. A.1. Diagram of One-Dimensional Reactor.

point 4 the fluxes are zero. For simplicity, let the mesh spacing be unity. The different materials of which the reactor is made are A, B, C. The constants of the materials are as follows:

	A	B	C
D_1	1.0	2.0	3.0
D_2	3.0	2.0	0
$\Sigma_{1\to2}$	0.1	0.2	0.3
$\Sigma_{2\to1}$	0	0	0
Σ_{A1}	2.0	0.2	0.3
Σ_{A2}	0.1	0.2	0.3
$\nu\Sigma_{f1}$	0.1	0.4	0.5
$\nu\Sigma_{f2}$	0	0	0.5
χ_1	1.0	1.0	1.0
χ_2	0	0	0

With these constants the difference equations for the reactor become (denoting fast fluxes by ϕ and slow ones by f):

$$2(\phi_3 - \phi_2) - \frac{1}{2}\,[0.1 + 0.2 + 2.0 + 0.2]\,\phi_2 + \frac{1}{k}\,[\tfrac{1}{2}(0.1 + 0.4)\,\phi_2] = 0\ ,$$

$$2(\phi_2 - \phi_3) + 3(-\phi_3) - \frac{1}{2}\,[0.2 + 0.3 + 0.2 + 0.3]\,\phi_3$$

$$+ \frac{1}{k}\,[\tfrac{1}{2}(0.4 + 0.5)\,\phi_3 + \tfrac{1}{2}(0.5)\,f_3] = 0\ ,$$

$$2(f_3 - f_4) - \frac{1}{2}\,[+\,0.1 + 0.2]\,f_4 + \frac{1}{2}\,[0.1 + 0.2]\,\phi_2 = 0\ ,$$

$$2(f_2 - f_3) + -\frac{1}{2}\,[+\,0.2 + 0.3]\,f_3 + \frac{1}{2}\,[0.2 + 0.3]\,\phi_3 = 0\ .$$

The matrices of the problem are:

$$A = \begin{vmatrix} 3.25 & -2 & 0 & 0 \\ -2 & 5.5 & 0 & 0 \\ -0.15 & 0 & 2.15 & -2 \\ 0 & -0.25 & -2 & 2.25 \end{vmatrix}$$

$$M = \begin{vmatrix} 0.25 & 0 & 0 & 0 \\ 0 & 0.45 & 0 & 0.25 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{vmatrix}$$

The forward and adjoint solutions to the problems

$$A\phi = \frac{1}{k}\,M\phi \text{ and } A^T\phi^+ = \frac{1}{k}\,M^T\phi^+$$

are:

$k = 0.2$

$\phi_2 = 1$	$\phi_2^+ = 0.41$
$\phi_3 = 1$	$\phi_3^+ = 0.335$
$f_2 = 1$	$f_2^+ = 1.0$
$f_3 = 1$	$f_3^+ = 1.075$

We shall now estimate the effect of changing Σ_{A2} in region B using Eq. (17). $\Sigma_{A2,B}$ is the Z in question, so that

$$\frac{\delta M}{\delta \Sigma_{A2,B}} = 0 \ ,$$

$$\frac{\delta A}{\delta \Sigma_{A2,B}} = \begin{vmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0.5 & 0 \\ 0 & 0 & 0 & 0.5 \end{vmatrix} .$$

Hence

$$\frac{\delta k}{k\,\delta \Sigma_{A2,B}} = -\,0.2 \times \frac{[0.41 \quad 0.335 \quad 1.0 \quad 1.075]\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0.5 & 0 \\ 0 & 0 & 0 & 0.5 \end{bmatrix}\begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}}{[0.41 \quad 0.335 \quad 1.0 \quad 1.075]\begin{bmatrix} 0.25 & 0 & 0 & 0 \\ 0 & 0.45 & 0 & 0.25 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}}$$

$$= -\,0.615727 \ .$$

If the change in $\Sigma_{A2,B}$ were, say, +0.02 then the change in k which is predicted is

$$\delta k = -\,0.615727 \times 0.2 \times 0.02 = -\,0.0024629 \ .$$

The exact change in k is −0.002345109 by direct computation. If the change in $\Sigma_{A2,B}$ were −0.02, the exact change in k would be +0.002593164. If we compute the average value of $\frac{\delta k}{k\,\delta \Sigma_{A2,B}}$ from these two numbers, we obtain −0.617284, to be compared with −0.615727 computed from perturbation theory.

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