Journal of Nuclear Energy, Vol. 27, pp. 553 to 558. Pergamon Press 1973. Printed in Northern Ireland

ON EXTRAPOLATED ENDPOINTS IN THE TWO-GROUP THEORY OF NEUTRON DIFFUSION

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(*Recieved* 29 *January* 1973)

Abstract—The use of an extrapolated-endpoint boundary condition in criticality calculations is discussed from the point of view of two-group neutron-transport theory. The use of a single Milne-problem extrapolated endpoint is justified, from the lowest-order approximation to the transport-theory result, only for certain values of the material properties of a bare multiplying slab.

1. INTRODUCTION

THE use of the Milne-problem extrapolated endpoint to define a boundary condition for one-speed diffusion-theory criticality calculations is common practice and can, in fact, be well justified from the lowest-order approximation to the corresponding transport-theory result, as discussed by MITSIS (1963). We wish to discuss here the analogous situation for the two-group model and to show that the use of a single Milne-problem extrapolated endpoint is justifiable for a subset of the physical parameters of interest.

The analysis here is based on the two-group neutron-transport equation which can be written as

$$\mu \frac{\partial}{\partial x} \mathbf{\Psi}(x, \mu) + \mathbf{\Sigma}\mathbf{\Psi}(x, \mu) = \mathbf{C}\int_{-1}^{1} \mathbf{\Psi}(x, \mu')\, \mathrm{d}\mu', \tag{1}$$

where the angular-flux vector has elements $\psi_1(x, \mu)$ and $\psi_2(x, \mu)$,

$$\mathbf{\Sigma} = \begin{bmatrix} \sigma & 0 \\ 0 & 1 \end{bmatrix}, \qquad \sigma = \frac{\sigma_1}{\sigma_2} > 1, \tag{2}$$

and, without loss of generality, the group transfer matrix $\mathbf{C}$, with positive elements c_{ij}, *is considered symmetric.* With regard to equation (1), we measure distances in terms of the optical variable x, and σ_1 and σ_2 are the two total cross-sections. As have KRIESE, SIEWERT and YENER (1973), hereafter referred to as KSY, we let

$$k_{\mathrm{BMS}} = \frac{1}{\sigma} c_{11} + c_{22} + \left[\left(\frac{1}{\sigma} c_{11} + c_{22}\right)^2 - \frac{4}{\sigma} \det \mathbf{C}\right]^{1/2} \tag{3}$$

and consider multiplying media to be defined by $k_{\mathrm{BMS}} > 1$. We thus seek, for $k_{\mathrm{BMS}} > 1$, that value of the slab half-thickness x_0 that permits a nontrivial solution of equation (1) subject to the conditions

$$\mathbf{\Psi}(-x, -\mu) = \mathbf{\Psi}(x, \mu) \quad \text{and} \quad \mathbf{\Psi}(x_0, -\mu) = \mathbf{O}, \quad \mu \in (0, 1). \tag{4}$$

As discussed by SIEWERT and SHIEH (1967), on seeking solutions of equation (1) of the form

$$\mathbf{\Psi}(x, \mu) = \mathbf{\Phi}(\nu, \mu)\mathrm{e}^{-x/\nu}, \tag{5}$$

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we find that two distinct cases must be considered: (i) $\kappa = 1$, which corresponds to one pair of discrete eigenvalues $\pm\nu_1$ and (ii) $\kappa = 2$, which corresponds to two pairs of discrete eigenvalues $\pm\nu_1$ and $\pm\nu_2$. We note that $\kappa = 2$ when the condition

$$c_{22} \leq 2 \det \mathbf{C} \operatorname{arctanh} \frac{1}{\sigma} \tag{6}$$

is satisfied. Further, we note that for $\kappa = 1$ *and* $k_{\mathrm{BMS}} > 1$ the eigenvalues are imaginary $\pm i\,|\nu_1|$; however, for $\kappa = 2$ *and* $k_{\mathrm{BMS}} > 1$ we can have either (a) an imaginary pair $\pm i\,|\nu_1|$ and a real pair $\pm\nu_2$ or (b) two imaginary pairs $\pm i\,|\nu_1|$ and $\pm i\,|\nu_2|$. For the sake of convenience, let us label the various possibilities as follows:

Case (1): $\kappa = 1$ and eigenvalues $\pm i\,|\nu_1|$, for $k_{\mathrm{BMS}} > 1$,

Case (2a): $\kappa = 2$ and eigenvalues $\pm i\,|\nu_1|$ and $\pm\nu_2$, $\nu_2 > 0$, for $k_{\mathrm{BMS}} > 1$,

Case (2b): $\kappa = 2$ and eigenvalues $\pm i\,|\nu_1|$ and $\pm i\,|\nu_2|$, for $k_{\mathrm{BMS}} > 1$.

2. ANALYSIS

We shall be concerned here principally with cases (2a) and (2b) since the critical problem for case (1) was recently discussed in KSY; however, the proof that a single endpoint is sufficient, for case (1), will be given. It was shown in KSY that the lowest-order transport-theory solutions, basic to a slab of half-thickness x_{00} and a sphere of radius r_{00}, for the two-group flux vectors were

$$\mathbf{\Phi}(x) = \mathbf{U}(\nu_1) \cos \frac{\pi x}{2(x_{00} + z_0)}, \quad \text{case (1)}, \tag{7a}$$

and

$$\mathbf{\Phi}(r) = \mathbf{U}(\nu_1) \frac{1}{r} \sin \frac{\pi r}{(r_{00} + z_0)}, \quad \text{case (1)}, \tag{7b}$$

where $\mathbf{U}(\nu_1)$ is a null-vector of $\mathbf{\Lambda}(\nu_1)$:

$$\mathbf{\Lambda}(\nu_1)\mathbf{U}(\nu_1) = \mathbf{0}, \tag{8}$$

with

$$\mathbf{\Lambda}(z) = \mathbf{I} + z \int_{-1}^{1} \mathbf{\psi}(\mu) \frac{d\mu}{\mu - z}, \tag{9}$$

$$\mathbf{\psi}(\mu) = \mathbf{\Theta}(\mu)\mathbf{C}, \qquad \mathbf{\Theta}(\mu) = \begin{bmatrix} \vartheta(\mu) & 0 \\ 0 & 1 \end{bmatrix}, \tag{10}$$

and $\vartheta(\mu) = 1$, $\mu \in (-1/\sigma, 1/\sigma)$, and $\vartheta(\mu) = 0$, otherwise. In addition, the lowest-order critical conditions are

$$x_{00} = \tfrac{1}{2}\pi\,|\nu_1| - z_0 \quad \text{and} \quad r_{00} = \pi\,|\nu_1| - z_0, \tag{11}$$

where z_0 is the extrapolated endpoint:

$$z_0 = -\frac{\nu_1}{2} \operatorname{Log} \left[\frac{1}{2} \frac{\nu_1}{N(\nu_1)} \tilde{\mathbf{U}}(\nu_1)\mathbf{C}\tilde{\mathbf{H}}^{-1}(\nu_1)\mathbf{C}^{-1}\mathbf{H}^{-1}(\nu_1)\mathbf{C}\mathbf{U}(\nu_1) \right]. \tag{12}$$

In equation (12) the superscript tilde denotes the transpose operation, Log is used to denote the principal branch of the log function, and $\mathbf{H}(z)$ is the $\mathbf{H}$ matrix discussed by SIEWERT, BURNISTON and KRIESE (1972), hereafter referred to as SBK. Naturally equations (7) and (11) are reasonable approximations only if equation (12) yields a real value of z_0, and since $\mathbf{H}(\nu_1)$ is complex, $k_{\mathrm{BMS}} > 1$, it is not at all obvious that equation (12) will, in fact, yield a real value of z_0. We can, however, give the required proof by showing that

$$\Delta_{11} = -\frac{1}{2}\frac{\nu_1}{N(\nu_1)}\tilde{\mathbf{U}}(\nu_1)\widetilde{\mathbf{CH}^{-1}}(\nu_1)\mathbf{C}^{-1}\mathbf{H}^{-1}(\nu_1)\mathbf{C}\mathbf{U}(\nu_1) \tag{13}$$

has unit modulus.

To develop the proof we first note that

$$N(\nu_1) = \nu_1^2\tilde{\mathbf{U}}(\nu_1)\mathbf{C}\frac{\mathrm{d}}{\mathrm{d}z}\mathbf{\Lambda}(z)\Big|_{z=\nu_1}\mathbf{U}(\nu_1) \tag{14}$$

and that the $\mathbf{H}$ matrix can be expressed in terms of a certain canonical solution $\mathbf{\Phi}_0(z)$ of a matrix Riemann problem. As discussed in SBK, we can write

$$\mathbf{H}(z) = \mathbf{C}\tilde{\mathbf{\Phi}}_0^{-1}(-z)\mathbf{D}^{-1}(-z)\tilde{\mathbf{\Phi}}_0(0)\mathbf{C}^{-1}, \qquad \kappa = 1, \tag{15}$$

where

$$\mathbf{D}(z) = \begin{bmatrix} 1 & 0 \\ 0 & \dfrac{\nu_1 - z}{\nu_1} \end{bmatrix}, \qquad \kappa = 1. \tag{16}$$

We note that $\mathbf{\Phi}_0(z)$ has the very important property that

$$\mathbf{\Phi}_0(z) = \overline{\mathbf{\Phi}_0(\bar{z})}, \tag{17}$$

where the bar is used to denote complex conjugation. We can now enter equations (14) and (15) into equation (13) to deduce [after using equation (42) of SBK] that

$$\Delta_{11} = (\pm)\frac{\tilde{\mathbf{U}}(\nu_1)\mathbf{\Phi}_0(-\nu_1)\begin{bmatrix}0\\1\end{bmatrix}}{\tilde{\mathbf{U}}(\nu_1)\mathbf{\Phi}_0(\nu_1)\begin{bmatrix}0\\1\end{bmatrix}}, \qquad \kappa = 1, \tag{18}$$

and thus we conclude, regardless of the $(\pm)$ uncertainty in equation (18), that $|\Delta_{11}| = 1$, since $\mathbf{U}(\nu_1)$ is real and $\mathbf{\Phi}_0(-\nu_1) = \overline{\mathbf{\Phi}_0(\nu_1)}$. It thus follows that equations (7) are valid approximations ($\kappa = 1$), and that they can be characterized by a single real extrapolated endpoint.

We now wish to consider that class of critical problems for which $\kappa = 2$, i.e., cases (2a) and (2b). Since the elementary solutions of equation (1) were reported by SIEWERT and ZWEIFEL (1966), we can first write the desired solution $\mathbf{\Psi}(x, \mu)$ as a superposition of these elementary solutions. After then invoking the necessary restrictions, as given by equation (4), on $\mathbf{\Psi}(x, \mu)$ we obtain a system of singular integral equations for the expansion coefficients, $B(\nu_2)$ and the two-vector $\mathbf{B}(\nu)$, $\nu \in (0, 1)$, required to complete the solution. Subsequently the two-group, half-range orthogonality relations reported by SIEWERT and ISHIGURO (1972) can be used to regularize the singular equations to obtain the following nonsingular equations:

$$\frac{1}{2}\left[1 - \Delta_{11} \exp\left(i2\frac{x_0}{|\nu_1|}\right)\right] \exp\left(-i\frac{x_0}{|\nu_1|}\right) + \Delta_{12} \exp\left(-2\frac{x_0}{\nu_2}\right) B(\nu_2) = \int_0^1 \mathbf{K}(x_0;\, \nu_1, \nu')\mathbf{B}(\nu')\, d\nu', \quad (19a)$$

$$\tfrac{1}{2}\Delta_{21} \exp\left(i2\frac{x_0}{|\nu_1|}\right) \exp\left(-i\frac{x_0}{|\nu_1|}\right) + \left[1 - \Delta_{22} \exp\left(-2\frac{x_0}{\nu_2}\right)\right] B(\nu_2) = \int_0^1 \mathbf{K}(x_0;\, \nu_2, \nu')\mathbf{B}(\nu')\, d\nu', \quad (19b)$$

and

$$\mathbf{B}(\nu) = \mathbf{F}(x_0;\, \nu_1, \nu_2, \nu) + \int_0^1 \mathbf{K}(x_0;\, \nu' \rightarrow \nu)\mathbf{B}(\nu')\, d\nu', \qquad \nu \in (0, 1), \quad (19c)$$

where

$$\Delta_{\alpha\beta} = -\frac{(-1)^{\alpha-\beta}}{N(\nu_\alpha)} \frac{\nu_\alpha \nu_\beta}{\nu_\alpha + \nu_\beta} \tilde{\mathbf{U}}(\nu_\alpha)\mathbf{C}\tilde{\mathbf{H}}^{-1}(\nu_\alpha)\mathbf{C}^{-1}\mathbf{H}^{-1}(\nu_\beta)\mathbf{C}\mathbf{U}(\nu_\beta), \qquad \alpha, \beta = 1 \text{ or } 2. \quad (20)$$

Since we shall not require here the explicit expressions for $\mathbf{F}(x_0;\, \nu_1, \nu_2, \nu)$, $\mathbf{K}(x_0;\, \nu_1, \nu)$, $\mathbf{K}(x_0;\, \nu_2, \nu)$ and $\mathbf{K}(x_0;\, \nu' \rightarrow \nu)$ they will not be listed; we note, however, that these quantities are regular and that they can be expressed in terms of the $\mathbf{H}$ matrix and other known functions, and thus are considered known.

Before discussing further the solution of equations (19), we observe that here the flux vector,

$$\mathbf{\Phi}(x) = \int_{-1}^{1} \mathbf{\Psi}(x, \mu)\, d\mu$$

takes the form

$$\mathbf{\Phi}(x) = \cos\frac{x}{|\nu_1|}\,\mathbf{U}(\nu_1) + 2B(\nu_2)e^{-x_0/\nu_2}\cosh\frac{x}{\nu_2}\,\mathbf{U}(\nu_2) + 2\int_0^1 \mathbf{B}(\nu)e^{-x_0/\nu}\cosh\frac{x}{\nu}\, d\nu, \quad (21)$$

where $\nu_2 > 0$ for case (2a) and $\nu_2 = i\,|\nu_2|$ for case (2b). Should we now wish to proceed rigorously, we would have to prove the existence of a unique solution to equations (19) and subsequently develop, say iteratively, the required numerical results. Our goal here, however, is to investigate the manner in which approximate solutions to equations (19) can be established and subsequently to develop boundary conditions that can be used with some degree of confidence in the considerably simpler P-1 or diffusion theory approximation of equation (1). If, by analogy with typical one-speed approximations in finite media, we ignore the contribution due to the continuous spectrum, by taking $\mathbf{B}(\nu) = \mathbf{0}$, $\nu \in (0, 1)$, then equations (19) reduce to

$$\frac{1}{2}\left[1 - \Delta_{11} \exp\left(i2\frac{x_0}{|\nu_1|}\right)\right] \exp\left(-i\frac{x_0}{|\nu_1|}\right) + \Delta_{12} \exp\left(-2\frac{x_0}{\nu_2}\right) B(\nu_2) = 0 \quad (22a)$$

and

$$\tfrac{1}{2}\Delta_{21} \exp\left(i2\frac{x_0}{|\nu_1|}\right) \exp\left(-i\frac{x_0}{|\nu_1|}\right) + \left[1 - \Delta_{22} \exp\left(-2\frac{x_0}{\nu_2}\right)\right] B(\nu_2) = 0. \quad (22b)$$

The principal point of this work is now to prove for case (2a) that equations (22), and the resulting flux vector, can be further approximated. On the other hand, for case (2b) we have not been able to justify further approximation of equations (22); in fact, though we have no proof that such further approximation can or cannot be justified, numerical computations (ISHIGURO, 1973) suggest that equations (22) cannot be further approximated for case (2b).

Let us first consider case (2a) and further approximate equations (22) by ignoring equation (22b) and taking $B(\nu_2) = 0$ in equation (22a). We thus conclude that

$$\mathbf{\Phi}(x) = \mathbf{U}(\nu_1) \cos \frac{\pi z}{2(x_{00} + z_0)}, \quad \text{case (2a)}, \tag{23}$$

where the critical condition is

$$x_{00} = \tfrac{1}{2}\pi\, |\nu_1| - z_0, \tag{24}$$

and z_0 is again given by equation (12). As for case (1), we must now argue for case (2a) that equation (12) yields a real value for the extrapolated endpoint, or alternatively we must again show that $|\Delta_{11}| = 1$. As discussed in SBK, the relationship between $\mathbf{H}(z)$ and $\mathbf{\Phi}_0(z)$, for $\kappa = 2$, is not the same as that given by equation (15). In fact to express $\mathbf{H}(z)$ in terms of $\mathbf{\Phi}_0(z)$, for $\kappa = 2$, we must know the so-called partial indices, which for $\kappa = 2$ could perhaps be either $\kappa_1 = 0$ and $\kappa_2 = 2$ or $\kappa_1 = \kappa_2 = 1$. However, for case (2a) we have been able to prove, on considering both possibilities for the partial indices, that $|\Delta_{11}| = 1$. The proof follows in a manner analogous to that discussed for $\kappa = 1$ and thus will not be given here. It now follows that equation (12) yields a real z_0 for case (2a) and thus that equations (23) and (24) are valid approximations for this case.

Considering now case (2b), we note that here we can show that $\kappa_1 = \kappa_2 = 1$, and thus we must use equation (67a) of SBK to relate $\mathbf{H}(z)$ to $\mathbf{\Phi}_0(z)$. However, we have been unable to prove that $|\Delta_{11}| = 1$, or $|\Delta_{22}| = 1$, and thus we cannot argue, for case (2b), that equations (22) can be further approximated, as they can for case (2a). In fact, numerical calculations (ISHIGURO, 1973) have indicated that $|\Delta_{11}| \neq 1$ and $|\Delta_{22}| \neq 1$, for case (2b), and therefore we have some evidence, though admittedly not proof, that further approximation of equations (22), in the manner considered, is not appropriate here. Though a proof is lacking, we conclude from numerical considerations that equation (12) yields a complex z_0 and thus that, for case (2b), a single extrapolated endpoint cannot be justified. Subsequently we take, for case (2b), equations (22) to be our lowest-order approximation and deduce, for this approximation, that the flux-vector can be written as

$$\mathbf{\Phi}(x) = \cos \frac{x}{|\nu_1|}\, \mathbf{U}(\nu_1) + \xi \cos \frac{x}{|\nu_2|}\, \mathbf{U}(\nu_2), \quad \text{case (2b)}, \tag{25}$$

where

$$\xi = \frac{1}{\Delta_{12}} \left\{ \Delta_{11} \exp \left[i x_{00} \left(\frac{1}{|\nu_1|} - \frac{1}{|\nu_2|} \right) \right] - \exp \left[-i x_{00} \left(\frac{1}{|\nu_1|} + \frac{1}{|\nu_2|} \right) \right] \right\}. \tag{26}$$

In addition, the critical condition here is the transcendental equation

$$\Delta_{11} \exp [2i(x_{00}/|\nu_1|)] + \Delta_{22} \exp [2i(x_{00}/|\nu_2|)] - \Delta \exp \left[2i x_{00} \left(\frac{1}{|\nu_1|} + \frac{1}{|\nu_2|} \right) \right] = 1, \tag{27}$$

where

$$\Delta = \Delta_{11}\Delta_{22} - \Delta_{12}\Delta_{21}. \tag{28}$$

In conclusion we note that BARAN (1968) has made, based on numerical work, several comments on extrapolated endpoints for nonmultiplying media, $k_{\mathrm{BMS}} < 1$. Here, however, we have considered the multiplying case, $k_{\mathrm{BMS}} > 1$, and have shown for cases (1) and (2a) that a single z_0, as given by equation (12), can be used with confidence to define the lowest-order transport-theory solutions to two-group critical problems for slabs (or spheres). On the other hand, we have concluded that a single extrapolated endpoint is not sufficient for case (2b), but rather we believe that equation (27) should be considered the lowest-order approximation of the critical condition.

In KSY the lowest-order approximation was shown, for several practical cases, to be quite accurate for case (1), and ISHIGURO (1973) has deduced similar conclusions from calculations based on equation (24) for case (2a) and equation (27) for case (2b).

Acknowledgements—The author would like to express his gratitude to Professor Dr. W. KOFINK and Universität Karlsruhe for their kind hospitality and partial support of this work.

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