AAEC/E288

AUSTRALIAN ATOMIC ENERGY COMMISSION

RESEARCH ESTABLISHMENT
LUCAS HEIGHTS

EVALUATION OF BOUNDARY CONDITIONS FOR THE HETEROGENEOUS REACTOR CODE SOS-1

by

I.J. DONNELLY

August 1973

ISBN 0 642 99589 3

AUSTRALIAN ATOMIC ENERGY COMMISSION

RESEARCH ESTABLISHMENT

LUCAS HEIGHTS

EVALUATION OF BOUNDARY CONDITIONS FOR THE HETEROGENEOUS REACTOR CODE SOS–1

by

I. J. DONNELLY

ABSTRACT

Methods of evaluating the monopole and dipole channel boundary conditions for the heterogeneous reactor code SOS–1 are reviewed and the accuracy of each method is analysed. A simple method of evaluating the dipole channel boundary conditions is proposed. It is accurate whenever the boundary conditions are insensitive to the energy spectrum of the flux at the channel boundary.

National Library of Australia card number and ISBN 0 642 99589 3

The following descriptors have been selected from the INIS Thesaurus to describe the subject content of this report for information retrieval purposes. For further details please refer to IAEA–INIS–12 (INIS: Manual for Indexing) and IAEA–INIS–13 (INIS: Thesaurus) published in Vienna by the International Atomic Energy Agency.

BOUNDARY CONDITIONS; CYLINDRICAL CONFIGURATION; DIPOLES; ENERGY SPECTRA; FUEL ELEMENTS; MATRICES; MODERATORS; MULTIGROUP THEORY; NEUTRON DIFFUSION EQUATION; NEUTRON FLUX; NEUTRONS; REACTOR CELLS; REACTOR CHANNELS; REACTOR KINETICS; REACTOR LATTICES; S CODES; SGHWR REACTOR

CONTENTS

1. INTRODUCTION

In recent years several computer codes have been developed using the heterogeneous method of reactor calculation. Bonalumi and Bozzola (1971) have reviewed this field comprehensively and an extensive list of relevant literature has been compiled by Auerbach (1970). This report is mainly concerned with the preparation of boundary conditions for the code SOS–1 (Burnand 1967) but also contains a brief introduction to the heterogeneous method for completeness.

The most commonly developed heterogeneous theory applies to a reactor which is conveniently described using cylindrical geometry. The reactor under consideration is separated into cylindrical channels containing fuel elements, control rods, etc. and a moderator region. Diffusion theory is assumed to hold in the moderator and the solution of the multigroup diffusion equations can be written down in terms of moderator cross sections, reactor geometry and arbitrary constants. These constants are evaluated by specifying boundary conditions at the channel-moderator interfaces whence the flux distribution in the moderator is obtained. Thus, the flux spectrum at the channel boundaries is known and the reaction rates and flux distribution in each channel may be obtained using results of the cell calculations from which the boundary conditions were evaluated.

The form taken by these boundary conditions depends on the type of heterogeneous theory for which they are required. Two theories exist, the Nordheim-Scalettar version in which the boundary conditions, commonly called γ-matrices, are related to the linear extrapolation lengths of the multigroup moderator flux at the channel boundary, and the Feinberg-Galanin version in which the boundary conditions are given by the response coefficients obtained by taking a channel surrounded by an infinite moderator (an open cell) and evaluating the flux at the channel surface due to a fixed source distribution at infinity. Naudet (1968) has shown that, in theory, these two methods are identical and that the boundary conditions can be transformed from one form to the other. However, the approach used for their evaluation often varies. The γ-matrices are most amenable to a single cell calculation which will often limit their accuracy to channels having a reactor flux spectrum similar to the cell spectrum, while the response coefficients, in a G group theory, are best evaluated using G open cell calculations which lead to values that are independent of the flux spectrum at the channel.

The code SOS–1 requires boundary conditions of the γ-matrix type. These boundary conditions fall into two categories:

(i) monopole terms which specify the neutron absorption and production in a channel and thus must be evaluated accurately, and

(ii) dipole terms which are related to the ability of neutrons to move through a fuel element and which are generally adequate if evaluated to within 10 per cent.

The methods of evaluating the monopole terms discussed here have been developed previously by several authors so they are described only briefly, while the conditions under which they are accurate are more fully investigated.

As the dipole terms only need to be evaluated to within 10 per cent, they have been treated in several ways in the past, some being more accurate than others. These methods are considered and a new one is developed and tested. The new method is found to be accurate as long as the boundary conditions are insensitive to the energy spectrum of the flux at the channel boundary.

Although it is not used in this report, the open cell technique is often mentioned and so the difference between a cell calculation and an open cell calculation will be briefly explained. Consider a regular infinite lattice of identical channels in a moderator. The contours of zero flux gradient divide the lattice into cells consisting of a channel surrounded by moderator. The boundary of each cell is often approximated by a circular cylinder. In a G group diffusion theory cell calculation there are G boundary conditions that need to be specified before the cell flux can be evaluated, and there are G linearly independent ways in which a set of G boundary conditions can

be specified. The conventional cell calculation generally uses a zero current condition for all groups, along with an eigenvalue search. One form of the open cell calculation consists of calculating the cell flux for each of the G linearly independent sets of boundary conditions. The flux in the cell can be obtained for arbitrary boundary conditions using these results.

The most common form of open cell calculation is that used to obtain the response function form of channel boundary conditions for use in the heterogeneous method. In this case the channel is surrounded by an infinite moderator, hence the name 'open cell'. The channel flux is calculated assuming a source in the moderator in group g and zero source in the other groups. This calculation is repeated for all values of g, thus giving G linearly independent sets of results. The flux inside the channel can then be related to an arbitrary flux outside the channel, the relationship being given by the response functions.

2. THE HETEROGENEOUS METHOD

The neutron flux distribution in the moderator of a reactor with cylindrical channels is derived and its dependence on the channel boundary conditions is given. For mathematical simplicity the reactor is taken to be infinite in the $\underline{z}$ direction with a radially infinite moderator. Auerbach (1967) has given a treatment of the more realistic case of finite moderator. Multigroup diffusion theory with G groups is used to evaluate the flux in the moderator. The following treatment is similar to that of Bonalumi and Bozzola (1971).

In an obvious notation the diffusion equations to be solved are

$$- D_g \nabla^2 \phi_g + \Sigma_g^t \phi_g = \sum_{g' \neq g}^{G} \Sigma_{g \leftarrow g'}^s \phi_{g'} \tag{1}$$

which can be written in matrix form as

$$- \underline{\underline{D}} \nabla^2 \underline{\phi} + \underline{\underline{\Sigma}} \underline{\phi} = \underline{0} \quad . \tag{2}$$

The treatment is simplified if the following transformation is made. Define a pseudo-flux $\underline{Q}$ by

$$\underline{Q} = \underline{\underline{C}} \underline{\phi} \tag{3}$$

so that

$$\nabla^2 \underline{Q} = \underline{\underline{\lambda}} \underline{Q} \tag{4}$$

with

$$\lambda_{gg'} = \lambda_g \delta_{gg'} = \kappa_g^2 \delta_{gg'} \quad . \tag{5}$$

The matrices $\underline{\underline{\lambda}}$ and $\underline{\underline{C}}$ are evaluated in Appendix A. The G coupled equations for ϕ_g have thus been transformed into G independent equations for Q_g. The one group pseudo-fluxes Q_g are then easily obtained and transformed back to the real fluxes ϕ_g.

Consider N channels in an infinite moderator. The pseudo-flux Q_g may be expanded in the moderator in the form

$$Q_g(\underset{\sim}{r}) = \sum_{i=1}^{N} \left[A_{ig}^0 K_0(\kappa_g t_i) + \sum_{\nu=1}^{\infty} \left[A_{ig}^{\nu 1} \cos(\nu \theta_i) + A_{ig}^{\nu 2} \sin(\nu \theta_i) \right] K_\nu(\kappa_g t_i) \right] \tag{6}$$

where $K_\nu(z)$ are Bessel functions, $\underset{\sim}{t}_i$ is the vector from the centre of the ith channel to the point $\underset{\sim}{r}$ and θ_i is the angle between $\underset{\sim}{t}_i$ and the x-axis. The geometry is shown in Figure 1. The terms A_{ig}^0, $A_{ig}^{\nu 1}$ and $A_{ig}^{\nu 2}$ are unknown constants to be determined by boundary conditions. This series expression for $Q_g(\underset{\sim}{r})$ is generally terminated after a few terms. In the monopole approximation $A_{ig}^{\nu 1} = A_{ig}^{\nu 2} = 0$ for $\nu \geqslant 1$ while the dipole approximation includes the terms with $\nu = 1$.

In the dipole approximation the pseudo-flux at the surface of the jth channel is expressed in the form

$$Q_g(\rho_j, \theta_j) = Q_g^0(\rho_j) + Q_g^{11}(\rho_j)\cos\theta_j + Q_g^{12}(\rho_j)\sin\theta_j \tag{7}$$

where ρ_j is the radius of the jth channel.

The relationship between $Q_g^\mu(\rho_j)$ and the unknown constants A_{ig}^μ may be obtained by using Bessel function addition theorems to expand the terms $K_0(\kappa_g t_i)$, $K_1(\kappa_g t_i)\cos\theta_i$ and $K_1(\kappa_g t_i)\sin\theta_i$ around the centre of the jth channel in terms of t_j and θ_j. Substitute these expansions into Equation(6), take $\underset{\sim}{r}$ on the surface of the jth channel and then integrate $Q_g(\underset{\sim}{r})$ with respect to $d\theta_j$, $\cos\theta_j\ d\theta_j$ and $\sin\theta_j\ d\theta_j$ $(0 \leqslant \theta_j \leqslant 2\pi)$. The results are then equated with the respective integrals of Equation (7). Relationships of the form

$$Q_g^0(\rho_j) = A_{jg}^0 K_0(\kappa_g \rho_j) + B_{jg}^0 I_0(\kappa_g \rho_j) \tag{8}$$

are obtained where B_{jg}^0 is a constant which contains the unknown A_{ig}^μ as well as terms depending on the reactor geometry. Similar expressions are found for $Q_g^{11}(\rho_j)$ and $Q_g^{12}(\rho_j)$. For a comprehensive derivation of these relationships see Auerbach (1967).

In the dipole approximation the flux at the surface of the jth channel is expressed in the form

$$\phi_g(\rho_j, \theta_j) = \phi_g^0(\rho_j) + \phi_g^{11}(\rho_j)\cos\theta_j + \phi_g^{12}(\rho_j)\sin\theta_j . \tag{9}$$

The expressions for the terms $\phi_g^\mu(\rho_j)$ are found from Equation (7) using $\underset{\sim}{\phi} = \underset{\sim}{\underset{\sim}{C}}^{-1}\ \underset{\sim}{Q}$.

It is apparent from Equation (6) that in a G group dipole treatment of N channels there are 3NG constants to be evaluated for the multigroup flux in the moderator to be uniquely determined. This can be done by specifying a boundary condition for each of the flux components $\phi_g^\mu(\rho_j)$. For source-free problems this leads to a set of 3NG homogeneous equations for 3NG unknowns A_{ig}^μ and so an eigenvalue k_{eff} which specifies the reactivity of the system is also obtained.

The Nordheim-Scalettar method uses boundary conditions of the form

$$\left.\frac{d\phi_g^\mu(r)}{dr}\right|_{r=\rho_j} = \sum_{g'=1}^{G}\left[\gamma_{gg'}^{\mu j} + \frac{1}{k_{eff}}\gamma_{f,gg'}^{\mu j}\right]\phi_{g'}^\mu(\rho_j) \tag{10}$$

where the terms $\gamma_{gg'}^{\mu j}$, and $\gamma_{f,gg'}^{\mu j}$, are parameters characteristic of the jth channel. The evaluation of these parameters is considered in the remainder of this report.

3. MONOPOLE BOUNDARY CONDITIONS

In this section only the monopole component of the flux, ϕ_g^0, is considered so the index 0 is omitted. From Equation (9) it is apparent that the monopole component of the flux is independent of azimuthal angle θ. It can therefore be evaluated using a circular cylindrical cell calculation with appropriate cell boundary conditions.

3.1 The γ^0 Parameters from Neutron Balance

A convenient way to evaluate the monopole parameters γ^0 is to use neutron conservation in a channel to obtain an expression for γ^0 in terms of the neutron cross sections and flux in the channel, and then perform a cell calculation to obtain these fluxes. The group g neutron leakage out of a channel of radius ρ is related to the neutron production in the channel by the equation

$$2\pi\rho j_g(\rho) = \pi\rho^2\left[\sum_{g'=1}^{G}\left[\frac{1}{k}\chi_g\,\overline{\nu\Sigma_{g'}^f} + \overline{\Sigma_{g\leftarrow g'}}\right]\overline{\phi_{g'}} - \overline{\Sigma_g^t}\,\overline{\phi_g}\right] \tag{11}$$

where $j_g(\rho)$ is the current density at the channel surface,

$$\bar{\Sigma} = \frac{\int_o^\rho \Sigma\, \phi(r)\, r dr}{\int_o^\rho \phi(r)\, r dr} \quad \text{and} \quad \bar{\phi} = \frac{\int_o^\rho \phi(r)\, r dr}{\int_o^\rho r\, dr} \quad .$$

Diffusion theory is used in the moderator, so Equation (11) may be expressed in the form

$$D_g^m \left.\frac{d\phi_g^{as}}{dr}\right|_{r=\rho+} = \frac{\rho}{2}\left[-\sum_{g'=1}^{G}\left[\frac{1}{k}\chi_g\,\overline{\nu\Sigma_{g'}^f} + \bar{\Sigma}_{g\leftarrow g'}\right]\frac{\bar{\phi}_{g'}}{\phi_{g'}^{as}}\,\phi_{g'}^{as} + \overline{\Sigma_g^t}\,\frac{\bar{\phi}_g}{\phi_g^{as}}\,\phi_g^{as}\right] \qquad (12)$$

where $\phi_g^{as} = \phi_g^{as}(\rho)$ is the asymptotic flux in the moderator at the channel moderator boundary and D_g^m is the moderator diffusion coefficient. The asymptotic flux corresponds to the diffusion flux in the moderator and identifying Equation (12) with Equation (10) leads to

$$\gamma_{gg'}^o = \left[-\bar{\Sigma}_{g\leftarrow g'} + \delta_{gg'}\,\bar{\Sigma}_g^t\right]\frac{\rho\,\bar{\phi}_{g'}}{2\,D_g^m\,\phi_{g'}^{as}} \qquad (13)$$

and

$$\gamma_{f,gg'}^o = -\chi_g\,\overline{\nu\Sigma_{g'}^f}\,\frac{\rho\,\bar{\phi}_{g'}}{2\,D_g^m\,\phi_{g'}^{as}} \quad . \qquad (14)$$

3.2 The Significance of the Asymptotic Flux

A cell calculation using diffusion theory gives all the quantities necessary to evaluate $\gamma_{gg'}^o$, including the flux $\phi_{g'}^{as}$ which is then just the flux at the channel moderator boundary. If transport theory is used for the cell calculation, the flux at the boundary can be separated into two components, an asymptotic component which corresponds to the diffusion flux and a transient component which becomes negligible a few mean free paths into the moderator. As diffusion theory is used to evaluate the moderator flux in the SOS–1 code, then it must be the asymptotic flux $\phi_{g'}^{as}(\rho)$ which is used in the definition of the $\gamma_{gg'}^o$ values. Figure 2 shows the thermal flux $\phi(r)$ in a reflected cell assuming a constant downscatter source in the moderator and evaluation using transport theory. The asymptotic or diffusion theory flux is also shown in the moderator. Consider two values of γ^o: γ_a^o evaluated from Equation (13) using $\phi^{as}(\rho)$ in the denominator and γ_b^o evaluated using $\phi(\rho)$ in the denominator. If these values are used with Equation (10) and the diffusion theory flux at $r = \rho$ to evaluate the current at the channel boundary, it is apparent that γ_a^o will give the correct value while γ_b^o will over-value the current entering the channel. This current is related to the channel flux, so use of γ_a^o will lead to the correct channel flux while use of γ_b^o will lead to the too large value illustrated in Figure 2. In typical cases the difference between $\phi^{as}(\rho)$ and $\phi(\rho)$ is of the order of a few per cent.

Two ways of obtaining $\phi^{as}(\rho)$ are now considered for the case of a cell calculation performed using transport theory.

First of all, the channel-moderator boundary may be taken to be in the moderator and several mean free paths from the fuel element – moderator boundary. At this radius the transient component of the flux is negligible and the flux values given by the cell calculation are the required values $\phi_g^{as}(\rho)$. This method has several drawbacks. As it includes a large amount of moderator in the channel, all energy groups except the first have a large source term coming from downscatter and the radial flux shapes become dependent on the environment in which the channel is placed, that is on the flux spectrum at the channel boundary. The γ^o parameters are then spectrum dependent; this counteracts the accuracy of the heterogeneous method unless an iteration procedure is performed for the calculation of the γ^o parameters for each channel so that they are evaluated

using the relevant flux environment of the cell. However, if G open cell calculations are used for the evaluation of the γ° parameters then they are independent of the flux spectrum and this definition of the channel radius can be useful. Another drawback is that this method cannot be applied to tight lattices in which the fuel elements are only a few mean free paths apart.

In the second method, the channel boundary is taken to be the physical fuel element - moderator one and diffusion theory is used to calculate the moderator flux in the cell under consideration, using results from the original transport theory cell calculation as boundary conditions. To be explicit, consider the pseudo-flux $Q_g(r)$ in the moderator of a cylindrical cell. Then

$$Q_g(r) = AI_o(\kappa_g r) + BK_o(\kappa_g r) \tag{15}$$

where A and B are arbitrary constants to be determined by Q_g satisfying two boundary conditions. For G groups there are 2 G arbitrary constants to be found for $\underline{Q}$ and hence $\underline{\phi}$ to be evaluated. For each group the boundary conditions can be taken to be any two of the following three terms derived from the original cell calculation:

(i) current through channel boundary,

(ii) current through cell boundary, and

(iii) total flux in moderator.

A full description of the application of various combinations of the above boundary conditions is given in Appendix B. Once $\underline{\phi}$ has been obtained then $\phi_g^{as}(\rho) = \phi_g(\rho)$. This method of obtaining the asymptotic flux has the advantage that corrections can be made for any departure from diffusion theory in the moderator. By requiring that the diffusion flux satisfies the conditions (i) – (iii) it is ensured from neutron balance that a cell calculation performed using diffusion theory in the moderator and Nordheim-Scalettar boundary conditions at the channel leads to the same eigenvalue and channel reaction rates as found in the original transport theory cell calculation. In energy groups for which diffusion theory is not a good approximation in the moderator, the asymptotic flux does not correspond to the diffusion or P_1 flux, but to the asymptotic part of the P_n flux with n being suitably large. P_n theory can be used to derive a diffusion coefficient which when used in the P_1 equation converts it to the asymptotic P_n equation. This diffusion coefficient should replace the conventional one in the diffusion equation when required.

3.3 The Accuracy of Evaluating γ° from Cell Calculations

The use of a conventional cell calculation with reflective boundary conditions to evaluate the γ° parameters leads to the correct values for use in an infinite lattice of similar elements. However, the heterogeneous method is generally required for the evaluation of small or non-uniform reactors and so it is necessary to consider whether the γ° parameters derived from a simple cell calculation are applicable to a channel in an arbitrary flux environment.

The definition of the γ° parameters given in Equations (13) and (14) is of the form

$$\gamma^\circ_{gg'} \quad \alpha \quad \frac{\bar{\Sigma}\,\bar{\phi}_{g'}}{\phi_{g'}(\rho)} \quad \propto \int_{\text{channel}} \Sigma\,(\phi_{g'}(r)/\phi_{g'}(\rho))\,dV \quad . \tag{16}$$

Thus $\gamma^\circ_{gg'}$ is constant if the radial variation of the channel flux in group g' is independent of the flux spectrum at the cell boundary. This criterion will be satisfied in varying degrees depending on the neutron cross sections and the size of the cell under investigation. Several comments concerning this point are now made. For convenience a three group structure consisting of a fast, a resonance and a thermal group is considered.

(i) The parameter $\gamma^{\circ}_{gg'}$ is independent of all boundary conditions if there is no source term in the channel for group g' and if diffusion theory is valid in the cell. This holds because the group g' channel flux then has only one possible radial shape, independent of its magnitude.

The channel source can be due to fission or inscatter from other groups. The fission source is always present in group 1 which means that the group 1 flux shape is spectrum dependent. However, due to the small absorption of fast neutrons in most fuel elements, the value of k_{eff} is found to be insensitive to small variations of the group 1 flux shape in the channel.

(ii) For no channel source in group g' and a cell requiring a transport theory treatment, the flux shape, and thus the values of $\gamma^{\circ}_{gg'}$ are insensitive to realistic variations of channel flux spectrum.

(iii) From the above it is apparent that if the neutron source in group g' in the channel is small, so that the channel flux is composed predominantly of neutrons that have come in from the moderator in group g', then the flux shape and hence $\gamma^{\circ}_{gg'}$ are insensitive to the channel flux spectrum.

(iv) If the reactor under consideration is large with a uniform lattice of similar channels, then the original cell calculation is applicable to all channels and the method is accurate, even when there is a large amount of downscatter in the channels. This case is also solvable by various cell homogenisation methods.

(v) There are cases in which the cell cross sections and size are such that none of the conditions quoted in paragraphs (i) to (iv) are satisfied and each individual $\gamma^{\circ}_{gg'}$ may be strongly spectrum dependent. However, it must be remembered that the boundary conditions used are of the form

$$\left.\frac{d\phi_g}{dr}\right|_{r=\rho} = \sum_{g'=1}^{G} \gamma^{\circ}_{gg'}\ \phi_{g'}(\rho) \quad . \tag{17}$$

Several γ° parameters may be involved in each boundary condition, so errors in the $\gamma^{\circ}_{gg'}$ terms due to the wrong cell environment having been used in their calculation may often cancel one another with the result that the boundary condition of Equation (17) remains accurate.

(vi) Finally, it should be noted that the $\gamma^{\circ}_{gg'}$ terms can be derived in such a way that they are independent of the flux spectrum at the channel. This means using the open cell technique. They are not then related to the neutron production and absorption in the channel as are the terms defined in Equations (13) and (14).

3.4 Cell Boundary Conditions

Various boundary conditions can be applied in a cell calculation. The most common one is the reflective boundary condition which simulates the cell surrounded by an infinite lattice of similar cells. This generally gives a reasonable approximation to the energy and spatial distribution of the flux as long as the eigenvalue $k_{\infty} \simeq 1$. This condition is often not met for fuel elements of small reactors for which a large value of k_{∞} leads to a distorted flux spectrum in the cell. For fuel elements containing little moderating material, the radial flux shape in the fuel in each group is independent of the flux environment, so the reflective cell calculation suffices for evaluation of the γ° parameters. However, the radial flux shape in fuel elements containing a large amount of moderating material does depend on the cell boundary conditions, so it is desirable to make these as realistic as possible. The code QUAVER (Allen 1967) uses semi-reflective boundary conditions in the analysis of such cells. Some idea is needed of the flux environment

surrounding the cell so an iteration procedure of cell evaluation →reactor calculation →new cell boundary conditions →cell evaluation, etc., may be necessary. If there is no cell code with adjustable boundary conditions available, then a possible approach is to perform a rough cell calculation, use this to homogenise the reactor core, surround the cell by this homogenised core and evaluate the flux in the cell. If necessary, this process can be iterated. The cell derived γ° values should be insensitive to small variation in the homogenised region surrounding the cell, and the one cell calculation then suffices for all elements of the same type in a similar flux environment. If this does not hold, then the variation of γ° with cell environment means that the open cell technique is the best one to use.

4. DIPOLE BOUNDARY CONDITIONS

4.1 Introduction

The ease with which neutrons can flow through a channel is related to the dipole boundary condition values, so the dipole terms have a direct effect on the flux leakage. Since the leakage term in general plays only a small part in the balance between the flux production and absorption in a reactor, then reactivity parameters such as k_{eff} are not as sensitive to dipole boundary conditions as they are to monopole ones. However, flux profiles across the reactor and the flux gradient across a channel may both change considerably with variations in the dipole terms. Thus the accuracy required for these terms depends on the phenomenon under investigation but, in most cases, errors of the order of 10 per cent are tolerable.

Several methods of evaluating the γ^{1} parameters are possible:

(i) The most accurate method is to use the open cell technique and P_n theory which lead to values of γ^{1} which are independent of channel environment. The major drawback with this method is that fairly complicated P_n theory computer codes are needed. As these codes are not available at AAEC, this method is not considered in this report; Auerbach (1967) gives specific details of this method.

(ii) A cell calculation may be carried out. This is complicated if transport theory is required since an angle-dependent source term is present and a two-dimensional calculation, or the evaluation of anisotropic collision probabilities, is necessary. Also, the choice of boundary conditions to be applied is not trivial. In diffusion theory the treatment simplifies and is similar to a conventional cell calculation. This case has been treated by Allen (1967) in the QUAVER code.

(iii) The most common method is to relate the diagonal parameters γ^{1}_{gg} to the homogenised cell radial diffusion coefficients, $\overline{D}_g$, using a relationship obtained by Blackburn and Griggs (1965) and to take the non-diagonal terms as zero. The accuracy of this approximation will be discussed.

(iv) A method is presented in this report in which the γ^{1} terms are evaluated using G one group calculations. The procedure is simple and fast, and from the experience obtained so far it is accurate enough for most applications.

4.2 The γ^{1} Parameters from Neutron Balance

The calculation of the dipole flux in a cell is related to the methods of evaluation of homogenised cell diffusion coefficients developed by Benoist (1964) and Leslie (1964). Bonalumi (1971) has reviewed the theory of homogenised cell diffusion coefficients; his treatment of the form of the dipole flux in a one group source dependent problem is summarised below.

Consider an infinite regular lattice of channels and let ϕ° be the lattice periodic flux produced by a lattice periodic source q. The flux surrounding a given channel that is produced by the tilted source qx (where the x-axis is orthogonal to the channel so that $x = r \cos\theta$), is

$$\begin{aligned}\phi^t(r,\theta) &= x\,\phi^\circ(\underset{\sim}{r}) - \xi(r,\theta) \\ &= [\,r\,\phi^\circ(\underset{\sim}{r}) - \xi^1(\underset{\sim}{r})\,]\cos\theta \\ &= \phi^1(\underset{\sim}{r})\cos\theta\ ,\end{aligned} \tag{18}$$

where $\xi(r,\theta) = \xi^1(\underset{\sim}{r})\cos\theta$ is the lattice periodic antisymmetric flux produced by the lattice periodic anisotropic source $\Omega_x\,\psi^\circ(\underset{\sim}{r},\underset{\sim}{\Omega})$, ψ° is the angular flux corresponding to ϕ°, and Ω_x is the x component of the vector $\underset{\sim}{\Omega}$. In the vicinity of the channel, the terms $\phi^\circ(\underset{\sim}{r})$ and $\xi^1(\underset{\sim}{r})$ have negligible θ dependence if $q(\underset{\sim}{r})$ is independent of θ. In general, this is true except near the edge of a lattice cell and it is this fact which allows cell cylindricalisation to be a good approximation. If $q(\underset{\sim}{r})$ is independent of θ then Equation (18) can be written as

$$\phi^t(r,\theta) = [\,r\,\phi^\circ(r) - \xi^1(r)\,]\cos\theta\ . \tag{19}$$

The tilted flux of Equation (19) is equivalent to the dipole flux term $\phi^{11}(r)\cos\theta$ of Equation (9) as both are proportional to $\cos\theta$.

It is apparent that, due to the direction dependent source $\Omega_x\,\psi^\circ$, a transport theory calculation of ξ^1 and hence ϕ^t is quite complicated. However, it simplifies in the diffusion approximation since only the scalar flux need be evaluated and as this is of the form $\phi^1(r)\cos\theta$ the differential equation satisfied by ϕ^t is one dimensional.

Consider now the balance equations for the dipole flux in the channel. The dipole flux in group g is taken as $\phi_g^1(r)\cos\theta$ and an integral of this flux over the volume of the channel is zero because of the factor $\cos\theta$. To obtain neutron balance equations the positive flux half of the channel ($-\pi/2 \leqslant \theta \leqslant \pi/2$) is considered. Equating current out of the channel with neutron production minus absorption gives

$$\begin{aligned}&\int_{-\pi/2}^{\pi/2} j_g^1(\rho)\cos\theta\,\rho\,d\theta + 2\int_0^\rho j_g^1(r,\pi/2)\,dr \\ &= \int_0^\rho \int_{-\pi/2}^{\pi/2}\left[\sum_{g'=1}^{G}\left[\frac{1}{k}\,\chi_g\,\nu\Sigma_{g'}^f + \Sigma_{g\leftarrow g'}\right]\phi_{g'}^1(r) - \Sigma_g^t\,\phi_g^1(r)\right]\cos\theta\,d\theta\,r\,dr\ .\end{aligned} \tag{20}$$

The terms $j^1(\rho)\cos\theta$ and $j^1(r,\pi/2)$ are the currents passing through the half channel surface at (ρ,θ) and $(r,\pi/2)$ respectively. They are shown in Figure 3.

Equation (20) reduces to the form

$$\begin{aligned}&j_g^1(\rho) + \frac{1}{\rho}\int_0^\rho j_g^1(r,\pi/2)\,dr \\ &= \frac{\rho}{2}\left[\sum_{g'=1}^{G}\left[\frac{1}{k}\chi_g\,\overline{\nu\Sigma_{g'}^{f1}} + \overline{\Sigma_{g\leftarrow g'}^1}\right]\overline{\phi_{g'}^1} - \overline{\Sigma_g^{t1}}\,\overline{\phi_g^1}\right]\end{aligned} \tag{21}$$

where

$$\overline{\Sigma^1} = \frac{\int_o^\rho \Sigma\, \phi^1(r)\, r\, dr}{\int_o^\rho \phi^1(r)\, r\, dr} \quad \text{and} \quad \overline{\phi^1} = \frac{\int_o^\rho \phi^1(r)\, r\, dr}{\int_o^\rho r\, dr} \quad .$$

Equation (21) for dipole flux balance is similar to Equation (11) for the monopole case except for the term $\int_o^\rho j^1(r, \pi/2)\, dr/\rho$. This term is easily evaluated in the following manner if diffusion theory is used.

Consider the one group diffusion equation

$$\nabla^2 \phi^t(\underset{\sim}{r}) - \kappa^2 \phi^t(\underset{\sim}{r}) = 0 \tag{22}$$

when $\phi^t(\underset{\sim}{r})$ is the dipole flux $\phi^1(r) \cos\theta$. Equation (22) becomes

$$\frac{d^2\phi^1}{dr^2} + \frac{1}{r}\frac{d\phi^1}{dr} - \left(\kappa^2 + \frac{1}{r^2}\right)\phi^1 = 0 \quad , \tag{23}$$

with the general solution

$$\phi^1(r) = A\, I_1(\kappa r) + B\, K_1(\kappa r) \quad . \tag{24}$$

The neutron current in direction $\underset{\sim}{\Omega}$ is given by

$$j^1(r, \theta) = \underset{\sim}{\Omega} \cdot [-D \underset{\sim}{\nabla} [\phi^1(r) \cos\theta]\ ]$$

$$= -\Omega_r D \frac{d\phi^1(r)}{dr} \cos\theta + \Omega_\theta D \frac{\phi^1(r)}{r} \sin\theta \, . \tag{25}$$

The current terms in Equation (21) thus have the form

$$j_g^1(\rho) = -D_g^m \left.\frac{d\phi_g^1}{dr}\right|_{r=\rho^+} \quad , \tag{26}$$

where the suffix m signifies moderator values, and

$$j_g^1(r, \pi/2) = \frac{D_g(r)}{r}\, \phi_g^1(r) \quad . \tag{27}$$

Equation (21) then becomes

$$D_g^m \left.\frac{d\phi_g^1}{dr}\right|_{r=\rho^+} = \frac{\rho}{2}\left[-\sum_{g'=1}^{G}\left[\frac{1}{k}\chi_g\, \nu\overline{\Sigma^f}^1_{g'} + \overline{\Sigma}^1_{g\leftarrow g'}\right]\frac{\overline{\phi}^1_{g'}}{\phi^1_{g'}(\rho)} \cdot \phi^1_{g'}(\rho)\right.$$

$$\left. + \left[\overline{\Sigma^t}^1_g + \left(\overline{\frac{D_g}{r^2}}\right)^1\right]\frac{\overline{\phi}^1_g}{\phi^1_g(\rho)} \cdot \phi^1_g(\rho)\right] \tag{28}$$

with

$$\left(\overline{\frac{D}{r^2}}\right)^1 = \frac{\int_o^\rho \frac{D(r)}{r^2}\, \phi^1(r)\, r\, dr}{\int_o^\rho \phi^1(r)\, r\, dr} \quad .$$

Hence the dipole flux boundary conditions can be expressed in the form

$$\left.\frac{d\phi^1_g}{dr}\right|_{r=\rho^+} = \sum_{g'=1}^{G} \left[\gamma^1_{gg'} + \frac{1}{k}\,\gamma^1_{f,gg'}\right] \phi^1_{g'}(\rho) \tag{29}$$

where

$$\gamma^1_{gg'} = \left[-\overline{\Sigma^1}_{g\leftarrow g'} + \delta_{gg'}\left[\overline{\Sigma^{t^1}_g} + \left(\frac{\overline{D_g}}{r^2}\right)^1\right]\right] \frac{\rho\,\overline{\phi^1_{g'}}}{2D^m_g \phi^1_{g'}(\rho)} \tag{30}$$

and

$$\gamma^1_{f,gg'} = -\chi_g\,\overline{\nu\Sigma^{f^1}_{g'}}\;\frac{\rho\,\overline{\phi^1_{g'}}}{2D^m_g \phi^1_{g'}(\rho)}\;. \tag{31}$$

Remember that the flux $\phi^1_g(r)$ in the above formulae refers to the radial part of the dipole flux and that the cross sections are averaged over the channel with $\phi^1_g(r)$ as the weighting function.

The above relations have been obtained assuming that the dipole flux is of the form $\phi^1(r)\cos\theta$. It could equally as well have been taken as $\phi^1(r)\sin\theta$ and a similar treatment would again lead to the relations in Equations (29)–(31). Thus, in the notation of Equation (9), any given channel has the same boundary conditions for the fluxes $\phi^{11}_g(r)$ and $\phi^{12}_g(r)$.

Finally it is emphasised that Equations (30) and (31) have been obtained under the assumption that diffusion theory holds in the cell.

4.3 Diagonal Representation of γ^1

For small channel radii, the dipole flux in the channel is well represented by a term of the form $\phi^1(r) = Ar$. Use of this relationship in Equations (30) and (31) shows that for small ρ

$$\gamma^1_{gg'} \propto \rho\,,\quad g \neq g' \quad \text{and} \quad \gamma^1_{gg} \propto \rho^{-1}\,.$$

Thus, in the limiting case $\rho \to 0$, only the diagonal boundary conditions are important. In general the diagonal term is dominant in any given group unless there is a large source term present and the channel radii are large. This fact led to the following simple prescription for the evaluation of the dipole boundary conditions (Blackburn and Griggs 1965). The non-diagonal terms ($\gamma^1_{gg'}$, $g \neq g'$) are taken as zero and the diagonal terms are defined in such a way that they are exact for a cell which has neither neutron absorption nor sources. The derivation of these diagonal terms is now considered.

Take a one group source free cylindrical cell with channel radius ρ, cell radius R and zero absorption. The radial part of the dipole flux satisfies Equation (23) with $\kappa = 0$ and so has the general solution

$$\phi^1(r) = Ar + B/r \tag{32}$$

in the moderator. A value of γ^1 satisfying the relationship

$$\left.\frac{d\phi^1}{dr}\right|_{r=\rho} = \gamma^1\phi^1(\rho) \tag{33}$$

is required. Using the usual flux weighting methods and Benoist diffusion coefficients the cell can be homogenised and the homogenised flux expressed in the form

$$\phi^h(r) = Cr\;. \tag{34}$$

Normalising the homogenised flux at the cell boundary, the current at the boundary is

$$-\bar{D}\,\nabla\,\phi^{h}(r)\Big|_{r=R} = -\bar{D}/R \qquad (35)$$

where $\bar{D}$ is the radial diffusion coefficient for the homogenised cell. The fact that the flux and current in the ordinary and homogenised cells must agree at the cell boundary can be used to evaluate the constants A and B in Equation (32); so, from Equation (33),

$$\gamma^{1} = \frac{1}{\rho}\,\frac{1+b}{1-b}, \quad b = \frac{R^{2}}{\rho^{2}}\,\frac{\bar{D}-D^{m}}{\bar{D}+D^{m}} \qquad (36)$$

where D^{m} is the moderator diffusion coefficient.

An investigation of the general case of the dipole flux in group g shows that the relationship given in Equation (36) is adequate as long as the source and absorption terms in the moderator tend to cancel each other so that the moderator flux can be expressed in the form given in Equation (32). Bridge and Howarth have developed an improvement in this treatment which has been reported by Bonalumi and Bozzola (1971). They make reasonable assumptions about the source distribution in each group and use the resulting equation for the moderator flux to derive the diagonal boundary conditions in the same way as in Equations (32) to (36). This method should prove sufficiently accurate in cases when the approximation of zero non-diagonal terms is adequate.

4.4 The RATIO Method

The $\gamma^{1}_{gg'}$ terms may be obtained from a multigroup cell calculation. As a special code is needed to obtain the dipole flux and hence the γ^{1} terms, the accuracy of evaluating the dipole flux using a single group approximation for each energy group has been examined. This has led to the RATIO method which is based on the observation that the ratio $\gamma^{1}_{gg'}/\gamma^{0}_{gg'}$ is insensitive to the assumptions made regarding the presence of sources in the derivation of $\phi^{0}_{g'}$ and $\phi^{1}_{g'}$.

Taking the case of a homogeneous channel, the channel fluxes

$$\phi^{0}_{g'}(r) = A_{0}I_{0}(\kappa_{g'}r) \text{ and } \phi^{1}_{g'}(r) = A_{1}I_{1}(\kappa_{g'}r) \quad , \qquad (37)$$

derived from a one group, source free, diffusion theory calculation are used to evaluate $\gamma^{0}_{gg'}$ (approx.) and $\gamma^{1}_{gg'}$ (approx.). If $\gamma^{0}_{gg'}$ (exact) is the value found from one of the methods given in Section 3, then a good estimate of $\gamma^{1}_{gg'}$ (exact) is given by

$$\gamma^{1}_{gg'}\ (\text{exact}) \simeq \gamma^{0}_{gg'}\ (\text{exact})\ \Gamma \qquad (38)$$

where

$$\Gamma = \frac{\gamma^{1}_{gg'}\ (\text{approx.})}{\gamma^{0}_{gg'}\ (\text{approx.})} = \frac{\int_{0}^{\rho}\left[1+\delta_{gg'}/\kappa_{g}^{2}\,r^{2}\right] I_{1}(\kappa_{g'}r)/I_{1}(\kappa_{g'}\rho)\,r\,dr}{\int_{0}^{\rho} I_{0}(\kappa_{g'}r)/I_{0}(\kappa_{g'}\rho)\,r\,dr} \qquad (39)$$

Note the different form that Γ takes for diagonal and non-diagonal terms. A channel consisting of more than one region can be treated in a similar way to the one region case.

The RATIO method is exact in the following two cases:

(i) The obvious case in which the assumptions made in deriving the value of $\gamma^1_{gg'}$ are correct, that is when the g' group flux is correctly given by diffusion theory and there are no source terms in the channel for group g'.

(ii) In the case in which $\kappa_{g'}\rho \to 0$ for all groups. The fluxes in each group normalised at the channel boundary are then

$$\phi^0_{g'}(r) = 1 \qquad \text{and} \qquad \phi^1_{g'}(r) = r/\rho \ ,$$

which are also given by the one group source free approximation.

To evaluate the accuracy of the RATIO method in the general case, several different approximations made in obtaining the γ(approx.) terms need to be considered.

4.5 The RATIO Method and Transport Theory

The values of γ(approx.) are found assuming diffusion theory to hold in the channel. This will not lead to accurate values of the fluxes ϕ^0 and ϕ^1 if transport theory is required. However, it is found that Γ is insensitive to whether diffusion or transport theory is used in the flux evaluations. To illustrate this, consider a natural uranium rod in an infinite D_2O moderator with a source of thermal neutrons at infinity. The values of γ^0, γ^1 and γ^1/γ^0 found using P_1 and P_3 theory are shown in Table 1 for several fuel rod radii. The P_3 values of γ^0 and γ^1 are taken from a report by Auerbach and Mennig (1967). It is apparent that although the $\gamma^1(P_1)$ values are generally 10 – 20 per cent too high, the ratio $\gamma^1(P_1)/\gamma^0(P_1)$ agrees with $\gamma^1(P_3)/\gamma^0(P_3)$ to better than 5 per cent, except for the smallest radius rod where it is about 10 per cent too high. Therefore, the RATIO method evaluates γ^1 well within the desired 10 per cent accuracy in this example.

4.6 Weakly Moderating Channels

The effect of the presence of sources on the accuracy of γ^1, calculated using the RATIO method, has been investigated for a wide range of combinations of channel cross sections and source distributions using the following technique.

Take a homogeneous channel of radius ρ in an infinite moderator. In cylindrical geometry the one group diffusion equation is

$$\frac{d^2\phi^\nu}{dr^2} + \frac{1}{r}\frac{d\phi^\nu}{dr} - \left(\kappa^2 + \frac{\nu^2}{r^2}\right)\phi^\nu = -S^\nu(r) \tag{40}$$

where $\nu = 0, 1$ corresponding to the monopole and dipole case respectively. Take the source term as

$$S^\nu(r) = \alpha^\nu S^\nu \frac{I_\nu(\kappa_s r)}{I_\nu(\kappa_s \rho)} \qquad r \leq \rho \ ,$$

$$S^0(r) = S^0 \qquad r > \rho \qquad \text{and} \qquad S^1(r) = S^1 r/\rho \qquad r > \rho \ , \tag{41}$$

to simulate the type of group sources found in multigroup calculations. By increasing the factor α^ν the source term in the channel is made more important. The channel fluxes resulting from these sources are found and used to evaluate the ratio $\gamma^1(\alpha^1)/\gamma^0(\alpha^0)$ which is then compared with the ratio $\Gamma = \gamma^1(0)/\gamma^0(0)$. This investigation has shown that $\gamma^1(\alpha^1)/\gamma^0(\alpha^0)$ is insensitive to variations in α except in the case of a highly absorbing channel ($\kappa\rho >> 1$) which has an appreciable channel source term. In this case Γ can be in error by up to 25 per cent for a channel situated in the flux environment of a bare reactor, with even greater errors for a reflected reactor environment.

Results for a D_2O moderated fuel element which contains a large amount of moderating material are given in Table 2. The cross sections and radii correspond to those of an unburnt HIFAR fuel element. The percentage difference between $\gamma^1(0)/\gamma^0(0)$ and $\gamma^1(\alpha^1)/\gamma^0(\alpha^0)$ is given for fast, resonance and thermal groups for the case $\alpha^0 = \alpha^1 = \alpha$ which simulates the cell being in the flux environment of a bare reactor. The fast group α has been taken as 5 since most of the channel flux comes from the fission source. In the resonance and thermal groups it has been taken as 1 which simulates a large amount of moderating material in the channel. From the table it is apparent that the non-diagonal values of $\gamma^1(0)/\gamma^0(0)$ are accurate to about 7 per cent or better while the more important diagonal terms are generally correct to within 4 per cent.

4.7 Strongly Moderating Channels

The RATIO method of evaluating γ^1/γ^0 by neglecting source terms has been found to be quite accurate as long as the channel is not highly absorbing with a large source term present. To cope with this exception a pseudo-absorption cross section may be defined and used in the derivation of the source free fluxes and ratio $\Gamma = \gamma^1(\text{approx.})/\gamma^0(\text{approx.})$ as follows.

The diffusion equation for the gth group flux is

$$- D_g\left[\frac{d^2\phi_g^\nu}{dr^2} + \frac{1}{r}\frac{d\phi_g^\nu}{dr} - \frac{\nu^2}{r^2}\phi_g^\nu\right] + \Sigma_g^t \phi_g^\nu = \sum_{g'=1}^{G}\left[\frac{1}{k}\chi_g \nu\Sigma_{g'}^f + \Sigma_{g\leftarrow g'}\right]\phi_{g'}^\nu \quad . \tag{42}$$

There are G coupled equations to be solved to obtain the flux ϕ_g^ν . Equation (42) can be written in the form

$$- D_g\left[\frac{d^2\phi_g^\nu}{dr^2} + \frac{1}{r}\frac{d\phi_g^\nu}{dr} - \frac{\nu^2}{r^2}\phi_g^\nu\right] + \Sigma_g^{\nu,ps}\phi_g^\nu = 0 \quad , \tag{43}$$

where

$$\Sigma_g^{\nu,ps}(r) = \Sigma_g^t(r) - \sum_{g'=1}^{G}\left[\frac{1}{k}\chi_g \nu\Sigma_{g'}^f(r) + \Sigma_{g\leftarrow g'}\right]\phi_{g'}^\nu(r)/\phi_g^\nu(r) \quad . \tag{44}$$

Thus the group g flux satisfies a one group source free diffusion equation with absorption cross section $\Sigma_g^{\nu,ps}$. However, as the cross section depends on fluxes in other groups it is not known until all group fluxes have been obtained. The monopole fluxes are known from the cell calculation made for the preparation of the monopole boundary conditions, so $\Sigma_g^{0,ps}$ may be evaluated. If the monopole and dipole flux spectra are the same in the channel then $\phi_g^0(r)/\phi_{g'}^0(r) = \phi_g^1(r)/\phi_{g'}^1(r)$ and from Equation (44), $\Sigma_g^{0,ps}(r) = \Sigma_g^{1,ps}(r)$. Using this assumption, Equation (43) may be solved for the dipole flux and hence the dipole boundary conditions $\gamma_{g'g}^1$. In practice, though, the cross section $\Sigma_g^{0,ps}(r)$, which is r dependent even for a homogeneous channel, is only evaluated approximately since $\phi_{g'}^0(r)/\phi_g^0(r)$ is taken as constant for a given channel zone. As the ratio γ^1/γ^0 is less sensitive to cross section variation than γ^1, the method adopted is to use the fluxes ϕ_g^0 and ϕ_g^1 evaluated from Equation (43) to obtain the ratio $\Gamma = \gamma^1(\text{approx.})/\gamma^0(\text{approx.})$ and substitute this into Equation (38) to find $\gamma^1(\text{exact})$.

This method relies upon the assumption that the monopole and dipole flux spectra are similar in the channel. For a large uniform lattice of fuel elements this condition requires that

$$\frac{\phi_g^0(r)}{\phi_{g'}^0(r)} \approx \frac{\phi_g^1(r)}{\phi_{g'}^1(r)} = \frac{r\phi_g^0(r) - \xi_g^1(r)}{r\phi_{g'}^0(r) - \xi_{g'}^1(r)} \tag{45}$$

and it is satisfied if $\xi_g^1(r)/r\,\phi_g^0(r) << 1$. This may not hold in general but, for the situation of large absorption and large source terms considered in this section, it can be shown that

$$\left|\frac{\xi_g^1(r)}{r\,\phi_g^0(r)}\right| \simeq \left|\frac{\Sigma_g^{0,ps}}{\Sigma_g^r}\right| << 1 \quad . \tag{46}$$

Hence, under the given conditions and in a uniform lattice $\Sigma_g^{1,ps} \simeq \Sigma_g^{0,ps}$ and this method leads to an accurate evaluation of the γ^1 parameters. A word of caution is needed here, however, since the dipole flux spectrum changes considerably for channels near a reflector. The above method may or may not then be adequate depending on whether or not there is a significant change in the shape of the dipole flux in the channel as the flux spectrum alters. If there is a large change then either an iteration procedure or the open cell technique is required for γ^1 evaluation.

4.8 Experience with the RATIO Method in Moderating Channels

As a test of the RATIO method for channels which have a large group to group scattering, it has been used to evaluate the dipole boundary conditions for an SGHWR type fuel element. The boundary conditions for the fuel element studied have been evaluated by Allen (1967) using the code QUAVER. The Σ^{ps} version of the RATIO method reproduces the γ^1 values with errors ranging from +14 per cent to −11 per cent, but in most cases less than 6 per cent. If the RATIO method is not used, but the γ^1 terms are calculated directly from Equations (30) and (31) using the one group diffusion theory fluxes from Equation (43), errors as high as 40 per cent are obtained. The QUAVER results have been obtained assuming similar cell boundary conditions for both the monopole and dipole fluxes which correspond in this case to a uniform lattice situation. Thus it is concluded that the RATIO method is adequate for the evaluation of dipole boundary conditions for a strongly moderating channel that is situated in the buckling mode flux environment characteristic of a uniform lattice.

The SOS–1 code has been used to analyse several SGHWR mock-up cores in the JUNO reactor (Briggs et al. 1968) to investigate the difference between the dipole flux spectrum of a channel near the core centre where a buckling mode holds and the spectrum of a channel near the reflector. Values of the monopole and dipole boundary conditions for a fuel element are given in Table 3. The dipole terms have been evaluated using the RATIO method and thus hold for a channel in a buckling mode flux. The dipole flux spectrum is found to vary quite markedly in the region of the reflector. At the edge of a central channel it is $\phi_1^1 : \phi_2^1 : \phi_3^1 \simeq 0.5 : 0.5 : 1$ while for a channel near the reflector it becomes $\phi_1^1 : \phi_2^1 : \phi_3^1 \simeq 3 : 3 : 1$. The effective boundary condition for the group 3 dipole flux at a central channel can thus be expressed as

$$\left.\frac{d\phi_3^1}{dr}\right|_{r=\rho} = [-.0369 \times 0.5 + 0.3909]\ \phi_3^1(\rho) = 0.3824\ \phi_3^1(\rho) \quad . \tag{47}$$

Assuming that the γ^1 parameters are spectrum independent, the boundary condition for a channel near the reflector becomes

$$\left.\frac{d\phi_3^1}{dr}\right|_{r=\rho} = [-.0369 \times 3 + 0.3909]\ \phi_3^1(\rho) = 0.2802\ \phi_3^1(\rho) \quad . \tag{48}$$

It appears, from this analysis, that a fixed diagonal value is not adequate for the dipole boundary condition in reflected assemblies. However, due to the large change in dipole spectrum at the reflector there is a change in the channel source strength for each energy group. This has the effect of altering the dipole flux shape in the channel and hence changing the γ^1 parameters. Estimates of the size of the changes in γ^1 values for channels near the reflector in the particular JUNO core studied, show that they would lead to a boundary condition for the thermal flux similar to that given in Equation (47). Thus, for this case, a full specification of spectrum independent

γ^1 parameters which accurately describe a channel in a uniform lattice leads to poorer boundary conditions near a reflector than does a diagonal approximation which satisfies the uniform lattice boundary conditions. Such a diagonal approximation would be given by Bridge and Howarth's modification of the Blackburn and Griggs method. However, this cannot be guaranteed to occur always and, due to the significant size of the off-diagonal dipole terms for strongly moderating fuel elements coupled with the large changes in dipole flux spectra that can occur, it is evident that either an iteration or an open cell procedure should be followed to obtain accurate values of the dipole flux boundary conditions and hence the flux distribution in non-uniform reactors when the channels are strongly moderating.

5. SUMMARY

The preparation of channel boundary conditions for heterogeneous reactor codes has been investigated with particular emphasis being placed on the Nordheim-Scalettar form which applies to the code SOS–1. Two types of boundary conditions need to be evaluated. There are the monopole terms, which determine the neutron absorption and creation in the channels, and there are the dipole terms, which determine the neutron current flowing through the channels.

Two different methods may be used for the preparation of the monopole boundary conditions. In the first a single multigroup cell calculation is carried out and the desired channel boundary conditions obtained. This may be done with computer codes available at AAEC and is of sufficient accuracy unless there are large group to group neutron transfers in the channels. In the latter case it may not be accurate when applied to very heterogeneous reactors unless an iteration procedure is used. The second method requires that G open cell calculations be carried out and this leads to boundary conditions which are independent of flux spectrum and therefore always accurate within the multigroup approximation. The relevant codes for this method are not at present available at AAEC.

The evaluation of dipole boundary conditions may also be carried out using multigroup cell calculations but, due to the asymmetric shape of the flux, this is difficult and is not done in general. Instead, use is often made of the fact that the diagonal terms of γ^1_{gg}, are generally dominant and that γ^1_{gg} is related to the gth group homogenised diffusion coefficient. An alternative method has been developed in this report. The full γ^1–matrix is evaluated using G one group diffusion theory calculations of the dipole flux. The resultant values are insensitive to whether or not diffusion theory is valid in the fuel channel.

The methods of preparation of boundary conditions for the heterogeneous reactor code SOS–1 investigated and developed in this report are adequate for the treatment of all channels except those in which the radial flux shape in the channel varies considerably with a change in flux spectrum at the channel surface. The boundary conditions for channels which fit into this category are best evaluated using the open cell technique.

6. REFERENCES

Allen, F.R. (1967). – AEEW – R 515.

Auerbach, T. (1967). – EIR – Bericht Nr. 100.

Auerbach, T. (1970). – EIR – Bericht Nr. 200.

Auerbach, T. and Mennig, J. (1967). – EIR – Bericht Nr. 115.

Benoist, P. (1964). – CEA R – 2278.

Blackburn, D. and Griggs, C.F. (1965). – ANL–7050 : 231.

Bonalumi, R.A. (1971). – Energia Nucleare 18 : 395.

Bonalumi, R.A. and Bozzola, S. (1971). – Energia Nucleare 18 : 271.

Briggs, A.J., Johnstone, I., Newmarch, D.A. and Kendall, K.C. (1968). – J. Brit. Nucl. Energy Soc. 7 : 125.

Burnand, G. (1967). – EIR – Bericht Nr. 126.

Leslie, D.C. (1964). – AEEW – M 292.

Naudet, R. (1968). – EACRP – L – 73.

TABLE 1

COMPARISON OF γ^0 AND γ^1 EVALUATED IN P_1 AND P_3 THEORY

Fuel Radius (cm)	$\gamma^0(P_1)$ (cm^{-1})	$\gamma^0(P_3)$ (cm^{-1})	$\gamma^1(P_1)$ (cm^{-1})	$\gamma^1(P_3)$ (cm^{-1})	$\frac{\gamma^1(P_1)}{\gamma^0(P_1)}$	$\frac{\gamma^1(P_3)}{\gamma^0(P_3)}$
0.5	0.095	0.089	1.10	0.91	11.5	10.2
1.0	0.18	0.16	0.64	0.56	3.55	3.53
2.0	0.29	0.24	0.45	0.38	1.51	1.59
3.0	0.36	0.29	0.42	0.36	1.18	1.22
4.0	0.38	0.32	0.42	0.36	1.09	1.11
5.0	0.40	0.34	0.42	0.37	1.05	1.07

Cross sections U : $\Sigma_a = 0.323\ cm^{-1}$, $\Sigma_{tr} = 0.719\ cm^{-1}$

D_2O: $\Sigma_a = 3.82 \times 10^{-5}\ cm^{-1}$, $\Sigma_{tr} = 0.397\ cm^{-1}$

TABLE 2

PERCENTAGE ERROR IN THE NON-DIAGONAL AND DIAGONAL VALUES OF THE RATIO $\gamma^1(0)/\gamma^0(0)$

Group	Σ^r (cm^{-1})	D (cm)	$\kappa\rho$	α	% Error in Non-Diagonal Term	% Error in Diagonal Term
Fast	0.02	1.54	0.59	5	5	1
Resonance	0.016	1.47	0.54	1	2	1
Thermal	0.04	0.95	1.07	1	7	4

The percentage error is given by

$$[\gamma^1(0)/\gamma^0(0) - \gamma^1(\alpha)/\gamma^0(\alpha)] \,/\, [\gamma^1(\alpha)/\gamma^0(\alpha)] \times 100\%$$

Fuel Rod Radius ρ = 5.2 cm

TABLE 3

MONOPOLE AND DIPOLE BOUNDARY CONDITIONS FOR AN SGHWR FUEL ELEMENT

	$\gamma^0_{gg'} + \gamma^0_{f,gg'}$			$\gamma^1_{gg'} + \gamma^1_{f,gg'}$		
g \ g'	1	2	3	1	2	3
1	0.0581	−0.0249	−0.1968	0.3849	−0.0161	−0.1582
2	−0.0658	0.0835	0	−0.0397	0.2508	0
3	0	−0.0563	0.1840	0	−0.0369	0.3909

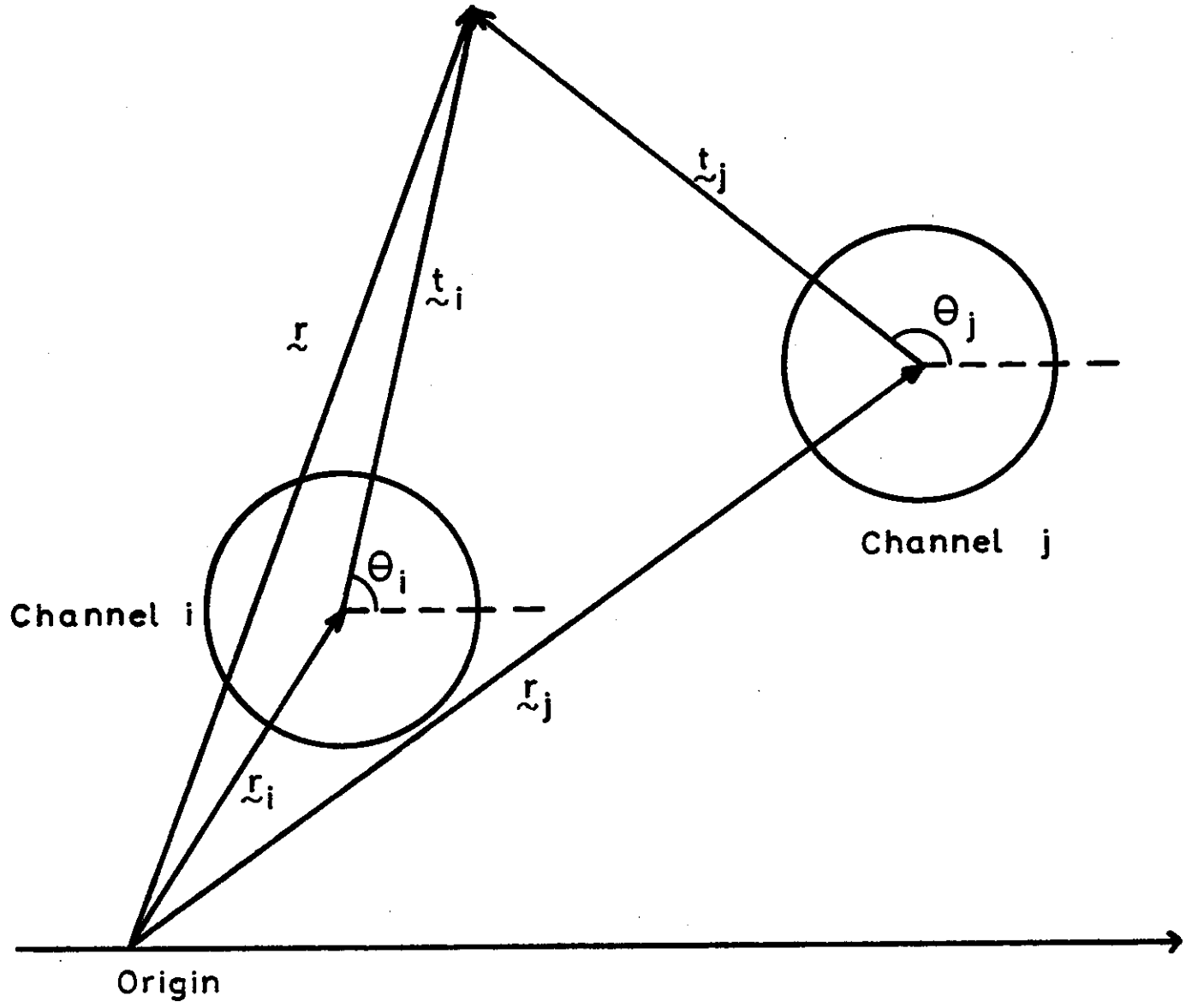
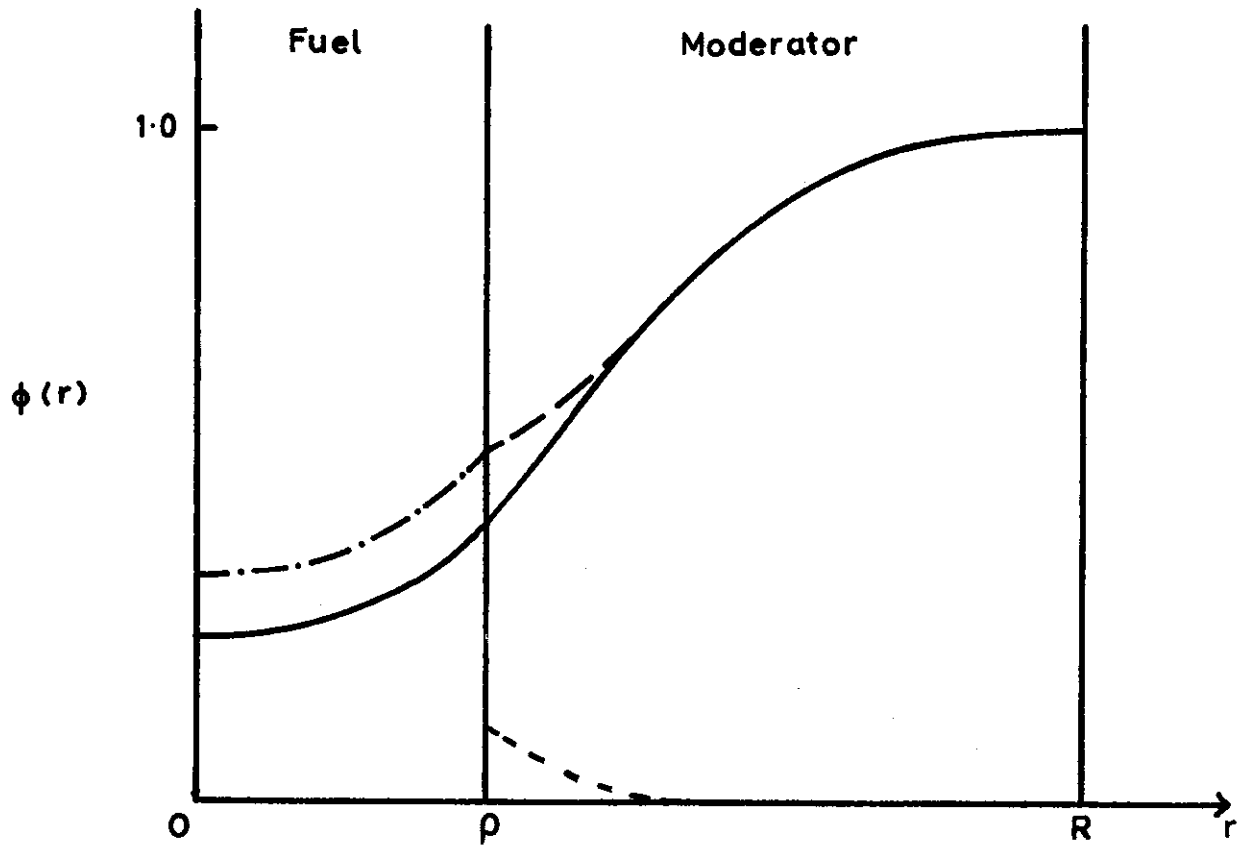


FIGURE 1. CO-ORDINATES OF POINT $\underset{\sim}{r}$ WITH RESPECT TO CHANNELS i AND j



Transport theory flux

Asymptotic component of moderator flux

Flux in fuel if $\phi(\rho)$ (instead of $\phi^{as}(\rho)$) is used to define γ°

(−1) x transient flux in moderator ($\phi^{as}(r) - \phi(r)$)

FIGURE 2. THE THERMAL FLUX IN A REFLECTED CELL

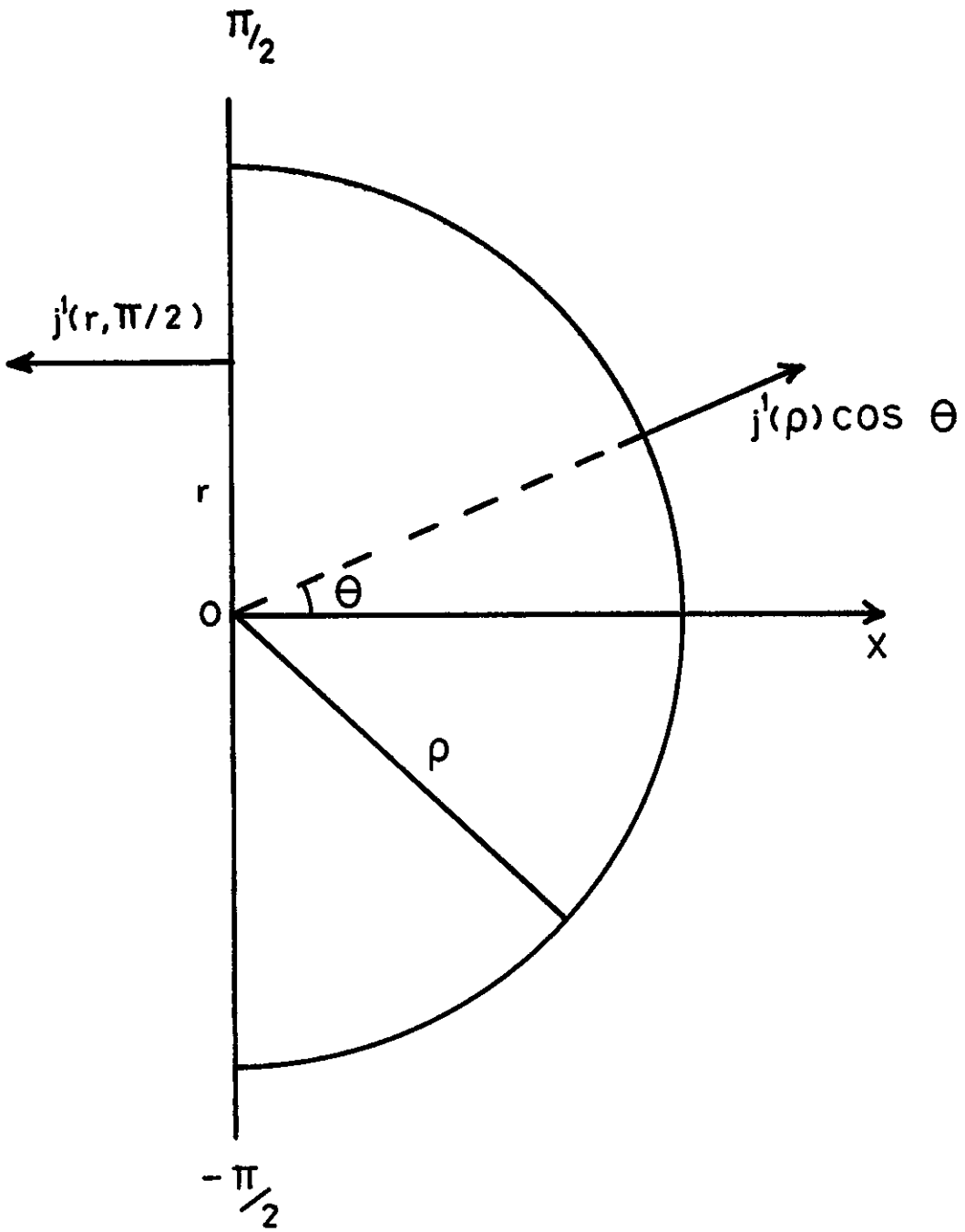


FIGURE 3. COMPONENTS OF THE DIPOLE CURRENT PASSING THROUGH THE HALF-CHANNEL SURFACE

APPENDIX A

DIAGONALISATION OF MULTIGROUP DIFFUSION EQUATIONS

In regions without fission sources the G group diffusion equations may be written in matrix notation as

$$-\underline{\underline{D}}\,\nabla^2\,\underline{\phi} + \underline{\underline{\Sigma}}\,\underline{\phi} = \underline{0} \tag{A1}$$

with

$$D_{ij} = D_i\,\delta_{ij}\ ,\ \Sigma_{ii} = \Sigma_i^r\ ,\ \Sigma_{ij} = -\Sigma_{i\leftarrow j}\quad i \neq j\quad . \tag{A2}$$

Define a pseudo-flux

$$\underline{Q} = \underline{\underline{C}}\,\underline{\phi} \tag{A3}$$

so that

$$\nabla^2\,\underline{Q} = \underline{\underline{\lambda}}\,\underline{Q} \tag{A4}$$

with

$$\lambda_{ij} = \lambda_i\,\delta_{ij} = \kappa_i^2\,\delta_{ij}\quad . \tag{A5}$$

It can be shown from Equations (A1), (A3) and (A4)

$$[\underline{\underline{D}}^{-1}\,\underline{\underline{\Sigma}}]^T\ \underline{\underline{C}}^T = \underline{\underline{C}}^T\,\underline{\underline{\lambda}} \tag{A6}$$

so that $\underline{\underline{C}}$ is a matrix whose rows are the eigenvalues of $[\underline{\underline{D}}^{-1}\ \underline{\underline{\Sigma}}]^T$ with eigenvalues $\{\lambda_i\}$.

The evaluation of $\underline{\underline{\lambda}}$ and $\underline{\underline{C}}$ becomes quite simple if there is no upscatter present since $\underline{\underline{\Sigma}}$ is then lower diagonal and the eigenvalues and eigenvectors are given immediately by

$$\lambda_i = \Sigma_i^r/D_i$$

$$C_{ij} = 0 \quad i < j$$

$$= 1 \quad i = j$$

$$= \frac{-\sum_{k=j+1}^{i} \Sigma_{k\leftarrow j}\,C_{ik}/D_k}{\lambda_i - \lambda_j} \quad i > j\quad . \tag{A7}$$

The components of the inverse matrix $\underline{\underline{C}}^{-1}$ are given by

$$C_{ij}^{-1} = 0 \quad i < j$$

$$= 1 \quad i = j$$

$$= \frac{\sum_{k=j}^{i-1} \Sigma_{i\leftarrow k}\ C_{kj}^{-1}/D_i}{\lambda_i - \lambda_j} \quad i > j\quad . \tag{A8}$$

Equation (A7) and Equation (A8), which are valid as long as $\{\lambda_i\}$ is not degenerate, lead to the immediate evaluation of $\underline{\underline{C}}$ and $\underline{\underline{C}}^{-1}$ without any matrix inversion.

APPENDIX B

EVALUATION OF ϕ^{as}

In Sections 3.1 and 3.2 it was shown that the asymptotic value of the flux at the channel boundary is required in the evaluation of γ°. The asymptotic component of the moderator flux is obtained from diffusion theory with the boundary conditions that the diffusion theory flux in each group has the same total value and the same current at the cell boundary as has the flux given by the original cell calculation.

The following equations for the asymptotic flux at the channel boundary are most easily derived by considering the pseudo-flux

$$Q_g(r) = A\, I_o(\kappa_g r) + B\, K_o(\kappa_g r) \quad . \tag{B1}$$

Evaluate A and B in terms of two of the three terms

$$\left.\frac{dQ}{dr}\right|_{\rho} \quad , \quad \left.\frac{dQ}{dr}\right|_{R} \quad \text{and } \overline{Q}$$

where ρ is the channel radius, R is the cell radius and $\overline{Q}$ is the average value of Q in the moderator. Thus an expression for $\underline{Q}(\rho)$ and hence $\underline{\phi}(\rho) = \underline{\phi}^{as}(\rho)$ can be obtained. Three alternative forms of this expression may be used depending on the two terms used to eliminate A and B in Equation (B1). All three lead to identical results.

Defining $\underline{\underline{Y}}$ and $\underline{\underline{Z}}$ as diagonal matrices, $a = \kappa_g \rho$, $b = \kappa_g R$ and $\alpha = I_1(b)\, K_1(a) - I_1(a)\, K_1(b)$,

the three equations are:

$$\text{(i)} \quad \underline{\phi}(\rho) = \underline{\underline{C}}^{-1}\, \underline{\underline{Y}}\, \underline{\underline{C}}\, \underline{\overline{\phi}} - \underline{\underline{C}}^{-1}\, \underline{\underline{Z}}\, \underline{\underline{C}} \left.\frac{d\underline{\phi}}{dr}\right|_{r = R} \tag{B2}$$

where

$$Y_{gg} = [\, I_o(a)\, K_1(b) + I_1(b)\, K_o(a)\,]\, [b^2 - a^2]\, /\, [2a\,\alpha] \quad ,$$

$$Z_{gg} = \left[[bI_1(b) - aI_1(a)]\, K_o(a) + [bK_1(b) - aK_1(a)]\, I_o(a)\right] / [\kappa_g a\, \alpha] \quad ,$$

$$\text{(ii)} \quad \underline{\phi}(\rho) = \underline{\underline{C}}^{-1}\, \underline{\underline{Y}}\, \underline{\underline{C}}\, \underline{\overline{\phi}} - \underline{\underline{C}}^{-1}\, \underline{\underline{Z}}\, \underline{\underline{C}} \left.\frac{d\underline{\phi}}{dr}\right|_{r = \rho^+} \tag{B3}$$

where

$$Y_{gg} = [I_o(a) K_1(a) + I_1(a) K_o(a)]\, [b^2 - a^2] / [2b\,\alpha] \quad ,$$

$$Z_{gg} = \left[[b\, I_1(b) - a\, I_1(a)]\, K_o(a) + [b\, K_1(b) - a\, K_1(a)]\, I_o(a)\right] / [\kappa_g\, b\, \alpha] \quad ,$$

$$\text{(iii)} \quad \underline{\phi}(\rho) = \underline{\underline{C}}^{-1}\, \underline{\underline{Y}}\, \underline{\underline{C}} \left.\frac{d\underline{\phi}}{dr}\right|_{r = \rho^+} - \underline{\underline{C}}^{-1}\, \underline{\underline{Z}}\, \underline{\underline{C}} \left.\frac{d\underline{\phi}}{dr}\right|_{r = R} \tag{B4}$$

where

$$Y_{gg} = -[I_o(a) K_1(b) + I_1(b) K_o(a)] / [\kappa_g \alpha] \quad ,$$

$$Z_{gg} = -[I_o(a) K_1(a) + I_1(a) K_o(a)] / [\kappa_g \alpha] \quad .$$

APPENDIX B (continued)

The terms

$$\left.\frac{d\phi_g}{dr}\right|_{r=\rho^+,R} = -D_g^{-1}\, j_g(\rho,R) \quad \text{and} \quad \bar{\phi}_g$$

are derived from the original cell calculation and substituted into Equations (B2) to (B4) to obtain $\phi_g(\rho)$. Note that in the case of a reflected cell

$$\left.\frac{d\phi_g}{dr}\right|_R = 0 \quad .$$