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CONTENTS

1 INTRODUCTION

In the practical application of nodal diffusion methods to light-water reactors, the reactor is partitioned into a number of large parallelepiped nodes (usually cuboids). Each of these nodes is assumed to have uniform homogeneous material properties and is typically of the size of a unit fuel assembly in the radial dimension, with similar (about 20 cm) axial dimensions. Historically, the ex-core reflector regions of a reactor have been modelled by means of albedo boundary conditions applied at the core periphery. The albedo boundary conditions are generally derived from very expensive higher-order calculations and are often empirically adjusted to give acceptable results. Modern nodal methods, on the other hand, are characterised by their ability to explicitly model these ex-core regions[1,2]. With these modern methods, albedo boundary conditions are usually no longer applied at the core periphery. There are several reasons for this.

Firstly, to derive accurate albedo boundary conditions for modelling the radial reflector, one must generally perform a two-dimensional (2-D) fine mesh reactor calculation with the ex-core regions explicitly (heterogeneously) represented. This defeats the inherent purpose of nodal methods.

Secondly, albedo boundary conditions are sensitive to changes in core conditions[3,4] and may have to be reevaluated as these conditions change. Although these sensitivities may not be large, they impair the considerable accuracy potential of modern nodal models[1]. This was not an important consideration with the older heuristic nodal models because of their limited accuracy capabilities. Moreover, these albedo boundary conditions were most probably partially responsible for the good accuracy of the old methods since

they could be used as adjustment parameters to compensate for the inherent deficiencies of these approximate methods.

Thirdly, most modern nodal models which are based on the transverse integration method calculate position–dependent transverse leakages for each node by utilising information on the nodal quantities calculated for its two nearest neighbour nodes in a given coordinate direction. Since the application of albedo boundary conditions on the core periphery would exclude obtaining information on the fluxes and transverse leakages within the ex–core regions, the calculation of the transverse leakage shapes in the peripheral fuel nodes becomes difficult and requires additional assumptions. This in turn negates the accuracy of these methods and is considered an unnecessary complication. This is one of the principal reasons for the explicit modelling of the ex–core regions in advanced nodal models.

In the explicit modelling of the ex–core regions in advanced nodal diffusion models, these regions are represented by homogeneous nodes of the same size as the core nodes. Since the ex–core regions can contain several structural material regions, as evidenced in the case of pressurised water reactor (PWR) radial reflectors, one is faced with the practical problem of obtaining homogenised cross sections for the ex–core nodes. This is a particularly serious problem in the case of PWR radial reflectors because of the presence of the steel baffle right next to the core. This steel baffle is a very good reflector of fast neutrons and a strong thermal absorber. A consequence of this is that strong flux gradients exist in the vicinity of the baffle and this causes the conventional flux–volume homogenisation method to fail badly when applied to PWR radial ex–core regions[3,4]. Even in the case of materially homogeneous reflector regions, the conventional method is not considered adequate because it cannot account for group collapsing errors and the significant transport effects that are prevailent in

these regions. The problem that the ex-core regions of a PWR thus poses to the reactor analyst is one of obtaining equivalent few-group diffusion theory constants that adequately account for homogenisation, group collapsing, and transport effects.

The Equivalence Theory (ET) developed by Koebke[5] provides an excellent solution to these problems since it is a rigorous and consistent homogenisation procedure. In fact, the homogenisation of the radial baffle/reflector regions of a PWR represents the most significant application of ET to PWR analysis[3]. Whereas the conventional homogenisation technique is adequate for homogenisation of the fuel assemblies of a PWR, it is most certainly not acceptable for the homogenisation of the steel baffle and reflector regions.

In this report we present an equivalent diffusion theory PWR reflector model which has as its basis Smith's generalisation[6] of Koebke's ET. Our method is an adaption, in one-dimensional slab geometry, of the Generalised Equivalence Theory (GET). It utilises the fact that the ratio of the so-called discontinuity factors on opposite sides of the common interface of two adjacent nodes is the only parameter important for conserving the neutronic coupling between these two nodes. Since the method involves the renormalisation of the GET discontinuity factors at nodal interfaces, it is called the Normalised Generalised Equivalence Theory (NGET) method.

As far as the layout of this report is concerned, the objective of this work is formulated in Section 2. This is followed by a short introduction to the notation used in this report. For the sake of completeness, the GET is first reviewed in Section 4 before the NGET is introduced in Section 5. The discussion of the GET draws heavily on Smith's recent review of advanced homogenisation techniques[3]. The definition of equivalent albedo boundary

conditions is presented in Section 7, and Section 8 summarises the advantages of the NGET method for modelling the ex–core nodes of a PWR. In Section 9 the application of the NGET to cell homogenisation problems is discussed. Section 10 considers guidelines for the practical determination of diffusion coefficients when conventional flux–volume weighting procedures are used. Conclusions are drawn in Section 11. The appendices detail the derivation of the analytic solution to the homogeneous diffusion equation as well as the derivation of certain response relations.

2 PROBLEM STATEMENT

The objective of this report is to present a consistent and rigorous method by which equivalent few–group diffusion theory constants can be obtained for the ex–core regions of a typical PWR. The conditions that the equivalent diffusion theory group constants are required to meet are:

(a) They should be applicable to modern nodal diffusion theory methods in which homogenised nodes of the size of a fuel assembly (in the radial dimension) are commonly used and in which only a few energy groups are generally considered.

(b) Because, in accordance with condition (a), these constants can at most be expected to conserve few–group volume integrated (node averaged) fluxes and reaction rates, and surface integrated (face averaged) net currents and fluxes, the nodal quantities to be conserved should be consistent with detailed multi–group transport theory predictions of the heterogeneous flux distribution in the ex–core regions of a PWR. Naturally, the transport theory predictions themselves must be physically realistic.

It would be advantageous if a single set of equivalent diffusion theory group constants could be found such that they are applicable to both nodal and conventional fine–mesh finite difference methods. Since this is most plausible in the case of the analytic diffusion theory nodal method, the particular method presented in this report is specifically designed for nodal methods in which the ex–core regions are treated analytically.

As far as the acceptability of a PWR reflector model is concerned, we emphasise the preservation of the few–group core leakages (net currents). Thus, we do not demand direct knowledge of the nodal fluxes and reaction rates in the ex–core nodes, even if they can be conserved. The neutronic interaction between the core and the (axial and radial) reflector regions of a PWR is, to a good approximation, of a one–dimensional nature. Because of this, it is assumed that multi–group transport theory solutions of 1–D slab models of the core and the ex–core regions of a PWR can be used as reference solutions for the calculation of equivalent few–group diffusion theory constants for the ex–core nodes. For practical reasons it is further assumed that core heterogeneities are unimportant for this purpose and that only a small part of the core (e.g. one assembly in the radial direction) needs to be modelled. From the results[4] obtained with the PWR reflector model developed in this report, it appears that the above assumptions are acceptable.

Since homogenised nodes in PWR analysis are typically cubic, or rectilinear in some cases, we shall restrict the following discussion to Cartesian geometries.

3 NOTATION

In this report we shall follow Weiss[12] and adopt the Dirac bra–ket notation. For brevity, we shall also make extensive use of matrix notation. As an

illustration, consider the angle-integrated multi-group transport equation in standard notation:

$$\nabla\cdot\underline{J}_g(r) + \Sigma_{tg}(r)\Psi_g(r) = \sum_{g'} \left[\Sigma_{sgg'}(r) + \frac{1}{\lambda}F_{gg'}(r)\right]\Psi_{g'}(r) \quad . \quad (g = 1,\ldots,N) \tag{1}$$

In matrix notation, this equation becomes:

$$\nabla\cdot\tilde{\underline{J}}(r) + \hat{\Sigma}_t(r)\tilde{\Phi}(r) = \left[\hat{\Sigma}_s(r) + \frac{1}{\lambda}\hat{F}(r)\right]\tilde{\Phi}(r) \quad . \tag{2}$$

In the above, $\underline{J}_g(r)$ is the group g net current vector (in space) and $\Psi_g(r)$ is the group g scalar flux at position r; $\tilde{\underline{J}}(r)$ and $\tilde{\Phi}(r)$ are column vectors having as elements the N group g currents and fluxes respectively; $\hat{\Sigma}_\alpha$ represents the square NxN matrix with elements $\Sigma_{\alpha gg'}$. It is assumed that the reader is familiar with the conventional notation and the meaning of the parameters used to describe the behaviour of neutrons in a nuclear reactor.

In bra-ket notation, Eq. (1) is written as:

$$\nabla\cdot\langle g|\underline{J}(r)\rangle + \langle g|\Sigma_t(r)|\Psi(r)\rangle = \langle g|\Sigma_s(r) + \frac{1}{\lambda}F(r)|\Psi(r)\rangle \quad , \tag{3}$$

where $\Sigma(r)$ indicates an operator. We say that Eq. (3) is the transport equation written in the group representation. The group representation is defined to have as its basis the set of group kets, $\{|1\rangle,|2\rangle,\ldots,|N\rangle\}$, where the group ket $|g\rangle$ is defined as an N-tuple,

$$|g\rangle \equiv (0,\ldots,0,1,0,\ldots,0) \quad , \tag{4}$$

with 1 in the g'th position. In other words, Eq. (3) merely depicts the transport equation written in a specific coordinate system (the group representation). The transport equation could also be written symbolically without any reference to a particular representation:

$$\nabla\cdot|\underline{J}(r)> + |\Sigma_t(r)|\Psi(r)> = |\Sigma_s(r) + \frac{1}{\lambda}F(r)|\Psi(r)> \quad . \tag{5}$$

Using this symbolic expression as starting point, it is easy to write the transport equation in any desired representation.

A particularly important operator which is central to the application of the bra–ket notation in the present work is the closure relation

$$\sum_{i=1}^{N} |\alpha_i><\bar{\alpha}_i| = E \quad . \tag{6}$$

Here E represents the identity operator, $|\alpha_i>$ represents a basis ket in the α–representation and $<\bar{\alpha}_i|$ represents the dual basis bra relative to this basis ket. The relationship between the basis bras and dual basis kets is:

$$<\bar{\alpha}_i|\alpha_j> = <\alpha_j|\bar{\alpha}_i> = \delta_{ij} \qquad (i,j = 1,\ldots,N) \quad . \tag{7}$$

The mathematical foundations of the Dirac bra–ket notation as applied to non–self–adjoint operators is explored in Reference 7. Hence other concepts and definitions, such as the reciprocal bases, images, inner and scalar products, modal matrices, etc., which are required to establish the Dirac bra–ket notation for application to neutron transport problems, can be found in Reference 7.

4 GENERALISED EQUIVALENCE THEORY

Consider a known reference multi-group (N groups) transport theory solution:

$$\nabla\cdot\tilde{\underline{J}}(r) + \hat{\Sigma}_t(r)\tilde{\Phi}(r) = \hat{\Sigma}_s(r)\tilde{\Phi}(r) + \frac{1}{\lambda}\hat{F}(r)\tilde{\Phi}(r) \quad . \tag{8}$$

We wish to solve the much simpler homogenised few-group (K groups) problem:

$$\nabla\cdot\tilde{\underline{J}}^{hom}(r) + \hat{\Sigma}_t^{hom}(r)\tilde{\phi}(r) = \hat{\Sigma}_s^{hom}(r)\tilde{\phi}(r) + \frac{1}{\kappa}\hat{F}^{hom}(r)\tilde{\phi}(r) \quad . \tag{9}$$

The angular dependence of the transport equation has been integrated out since we are in practice usually not interested in this angular dependence.

Integrating both of the above equations over the volume of a given homogenisation region (node) and integrating just the first equation over broad energy ranges, and demanding term by term equivalence, defines an equivalent homogenised problem. For convenience, we also demand equivalence of the node average fluxes. The homogenised problem is thus said to be equivalent to the heterogeneous reference problem if:

$$\int_{S_{ik}} \langle G|\underline{J}^{hom}(r)\rangle\cdot\underline{n}_{ik}dS = \sum_{g\in G}\int_{S_{ik}} \langle g|\underline{J}(r)\rangle\cdot\underline{n}_{ik}dS = S_{ik}\langle G|J_{nik}\rangle \quad ;$$

$$\int_{V_i} \langle G|\Sigma_\alpha^{hom}(r)|G'\rangle\langle G'|\phi(r)\rangle dr = \sum_{g\in G,g'\in G'}\int_{V_i} \langle g|\Sigma_\alpha(r)|g'\rangle\langle g'|\Psi(r)\rangle dr; \tag{10}$$

$$\kappa = \lambda \quad ;$$

$$\int_{V_i} \langle G|\phi(r)\rangle dr = \sum_{g\in G}\int_{V_i} \langle g|\Psi(r)\rangle dr = V_i\langle G|\phi^{av}\rangle = V_i\langle G|\Psi^{av}\rangle \quad .$$

Here V_i is the volume of node i, S_{ik} the area of surface k of node i, and $\underline{n}_{ik}$ the outward unit vector normal to surface S_{ik}. Thus, $<G|J_{nik}>$ is the reference surface averaged net normal outgoing current across face k of node i in broad–group G; $<G|\Psi^{av}>$ is the node average flux in broad–group G. Note that α indicates a general cross section type.

If we define spatially constant homogenised cross sections within each node, the equivalent few–group cross sections are given by:

$$<G|\Sigma_\alpha^{hom}|G'> = \frac{\sum_{g\in G, g'\in G'} \int_{V_i} <g|\Sigma_\alpha(r)|g'><g'|\Psi(r)>dr}{\sum_{g'\in G'} \int_{V_i} <g'|\Psi(r)>dr} \quad . \tag{11}$$

If we further assume the equivalent homogenised problem to be described by the conventional diffusion equation, that is,

$$\tilde{\underline{J}}^{hom}(r) = -\hat{D}(r)\nabla\tilde{\phi}(r) \quad , \tag{12}$$

then we have, for each face k of node i (assuming node–wise position–independent D's),

$$<G|D_{ik}|G> = \frac{-\sum_{g\in G} \int_{S_{ik}} <g|\underline{J}(r)>\cdot\underline{n}_{ik}dS}{\sum_{g\in G} \int_{S_{ik}} <g|\nabla\phi(r)>\cdot\underline{n}_{ik}dS} \quad . \tag{13}$$

This introduces a non–linear definition for the equivalent few–group diffusion coefficient by virtue of the fact that the equivalent homogeneous flux solution is

strongly coupled to the homogenised cross sections and diffusion coefficients. A similar non–linear definition for the cross sections is avoided by the demand for equivalence of the node average fluxes. It should also be noted that Eq. (13) does not guarantee positive group diffusion coefficients. This possibility, together with the non–linearity of the definition of face–dependent diffusion coefficients, renders Eq. (13) undesirable for defining an equivalent homogenised problem. Other means of obtaining equivalent diffusion theory parameters are therefore preferred.

In conventional homogenisation methods, the flux–volume weighted (FVW) cross sections calculated according to Eq. (11) are used together with few–group diffusion coefficients obtained from, for instance, the FVW total cross sections or the FVW inverse total cross sections. We note that 3+k essential nodal quantities (total, scattering and fission reaction rates, and k surface integrated net normal currents) must be conserved by an equivalent reactor problem. However, conventional FVW homogenisation permits only 3+1 free parameters (only one set of group diffusion coefficients is defined for all nodal faces). The conventional FVW homogenisation technique attempts only to conserve integral reaction rates but not surface leakages, and therefore does not contain a sufficient number of degrees of freedom to define an equivalent homogenised problem.

Koebke[5] realised that the conventional FVW cross sections and diffusion coefficients could define an equivalent homogenised problem if the usual requirement that the homogeneous flux solution be continuous everywhere is abandoned. Actually, there is absolutely no physical reason why the homogenised flux should be continuous everywhere, especially across interfaces between dissimilar nodes. This allowance for flux discontinuity introduces the extra degrees of freedom required to define an equivalent reactor problem.

Koebke's homogenisation theory, which is known as the Equivalence Theory (ET), was generalised by Smith[6]. The Generalised Equivalence Theory (GET) encompasses the ET as well as the NGET developed in this report.

To illustrate the fundamentals of this theory, we recall that the equivalent homogenised problem is required to conserve, in addition to volume integrated reaction rates and fluxes, the net normal currents integrated over individual nodal interfaces. This leads to the conclusion that one needs to consider only one coordinate direction at a time to determine the equivalent parameters that are additional to the FVW cross sections (i.e. the extra degrees of freedom). In correspondence with the transverse integration procedure used in most modern nodal methods, one then integrates the homogeneous neutron balance equation Eq. (9) combined with Eq. (12) over all coordinate directions (w) transverse to the particular one being considered (u). Then, for a given node i with constant FVW cross sections determined according to Eq. (11), one has:

$$-\hat{D}_i \nabla_u^2 \tilde{\bar{\phi}}_i(u) + \hat{\Sigma}_{ti}^{hom} \tilde{\bar{\phi}}_i(u) = \left[\hat{\Sigma}_{si}^{hom} + \frac{1}{\kappa}\hat{F}_i^{hom}\right] \tilde{\bar{\phi}}_i(u) - \tilde{L}_i^{hom}(u) \quad , \tag{14}$$

where

$$\tilde{\bar{\phi}}_i(u) = \frac{1}{A_{iu}} \int_{A_{iu}} \tilde{\phi}(r) dS \quad , \tag{15}$$

$$\tilde{L}_i^{hom}(u) = -\hat{D}_i \frac{1}{A_{iu}} \sum_w \int_{A_{iu}} \nabla_w^2 \tilde{\phi}(r) dS \quad . \tag{16}$$

A_{iu} represents the nodal area normal to direction u.

If the transverse leakage, $\tilde{L}_i^{hom}(u)$, is assumed known, then Eq. (14), with the reference eigenvalue λ substituted for κ, can be solved as an inhomogeneous

boundary value problem with the reference broad-group surface averaged net currents at the node boundaries in the u direction as boundary conditions. This would conserve all the required nodal quantities necessary to have an equivalent homogeneous flux solution in node i. In this regard it is of interest to note that the definition of the diffusion coefficient is still quite arbitrary and that the use of a FVW diffusion coefficient is merely convenient. Section 10 deals with those aspects that are important for the calculation of FVW diffusion coefficients.

The FVW cross sections, the imposed face averaged broad-group net currents and reference eigenvalue, together with the assumed known homogeneous transverse leakage shape, define a unique flux solution to the equivalent homogeneous problem for node i. Since the flux solution for a given node is directly dependent on the values of the group diffusion coefficients (and the cross sections) of the node, the equivalent homogeneous interface fluxes at the common interface of two adjacent nodes will in all probability be different. An inevitable result of this is that the equivalent face averaged homogeneous fluxes at nodal interfaces will not be equal to the face averaged broad-group reference heterogeneous fluxes at these interfaces. The different homogeneous interface fluxes for nodes i and i+1 (in the u direction) can be expressed in terms of the physically continuous heterogeneous (reference) interface flux by (u- indicates the left side of a node in the u direction):

$$\hat{f}_i^{u+}\,\tilde{\phi}_i^{u+} = \hat{f}_{i+1}^{u-}\,\tilde{\phi}_{i+1}^{u-} = \tilde{\psi}_{i+1}^{u-} = \tilde{\psi}_i^{u+} \quad , \tag{17}$$

where the diagonal "discontinuity factor" matrices are defined by:

$$\langle G|f_i^{u+}|G\rangle = \frac{\langle G|\psi_i^{u+}\rangle}{\langle G|\phi_i^{u+}\rangle} \quad ; \quad \langle G|f_{i+1}^{u-}|G\rangle = \frac{\langle G|\psi_{i+1}^{u-}\rangle}{\langle G|\phi_{i+1}^{u-}\rangle} \quad . \tag{18}$$

In the above, $\tilde{\phi}_i^{u\pm} = \tilde{\phi}_i(u\pm)$ and

$$<G|\psi_i^{u\pm}> = <G|\psi_i(u\pm)> = \frac{1}{A_{iu}} \sum_{g\in G} \int_{A_{iu}} <g|\Psi(r)>dS \Big|_{u\pm} \qquad (19)$$

Thus, while continuity of homogeneous net currents is postulated, the equivalent homogeneous fluxes are permitted to be discontinuous by a factor $\hat{f}_i^{u+}/\hat{f}_{i+1}^{u-}$ at the interface between nodes i and i+1. This is the essence of the GET. A diagonal discontinuity factor (DF) matrix is defined for each inner face of a node and a single $\hat{D}_i$ is defined for the homogenised node. Thus, GET has one more equivalent parameter (the $\hat{D}_i$) than actually required to define an equivalent homogenised problem. The ET differs from the GET in this respect. In ET, the fact that the diffusion coefficient matrix is arbitrary and can be used as a free parameter to define an equivalent homogenised problem is utilised. Consequently, Koebke[5] defines a single discontinuity factor matrix ($\hat{f}_i^u$) for both (opposite) faces in a particular coordinate direction by iteratively adjusting the $\hat{D}_i$ until the two opposite discontinuity factor matrices are equal. Since the resultant discontinuity factor matrix may be quite different from either one of the original GET discontinuity factor matrices on the two opposite faces, it is called a heterogeneity factor (HF) matrix. The ET is further characterised by the fact that directional diffusion coefficient matrices ($\hat{D}_i^u$) are introduced as equivalent parameters.

Relative to GET, the ET has the advantage that it effectively reduces the number of equivalent homogenised parameters to exactly the number necessary to define an equivalent homogenised problem. It has the disadvantage that it requires an iterative process to obtain the heterogeneity factors and that nodal codes must be able to use directional diffusion coefficients. It should also be noted that it may not be possible to determine a single (unique) real-valued $\hat{D}_i^u$

from the iterative process using the condition that $\hat{f}_i^{u-} = \hat{f}_i^{u+}$, especially for symmetric nodes. In order for the iterative prccedure to work, zero face averaged net leakages on the two opposite sides in the u direction must always be avoided, and for symmetric nodes an asymmetric leakage tilt in the u direction is also required. The extra degree of freedom of the GET circumvents these problems. In the case of asymmetric nodes, it has been shown that ET can fail to reproduce a known reference heterogeneous calculation[3]. This is due to the fact that ET guarantees a symmetric response matrix for a homogenised node, whereas GET does not. Another practical difficulty with ET is that the iterative procedure may yield undesirable negative group diffusion coefficients or HF's. The GET exhibits a similar difficulty with regard to the DF's: for a given arbitrary $\hat{D}_i$, negative $\tilde{\phi}_i^{\pm}$ may be obtained from the solution of the two–point boundary value problem for node i. We have encountered this problem in the case of homogenised PWR baffle/reflector nodes using FVW transport cross sections, or transport matrices. Fortunately, this is easily remedied by selecting another arbitrary $\hat{D}_i$ (see Section 7).

The preceding arguments relied on the prior knowledge of the magnitude and spatial shape of the equivalent homogeneous transverse leakage term, $\tilde{L}_i^{hom}(u)$. Since the 1–D NGET method, which is discussed in the next section, is the central issue of this report, this transverse leakage term is of no direct interest to us. However, to maintain generality as far as possible, we briefly discuss the significance of this term with regard to the solution of the two–point boundary value problem for the equivalent transverse integrated homogeneous flux.

Since the homogeneous transverse leakage term cannot be expected to have the same spatial fine structure as the heterogeneous transverse leakage, $\tilde{L}_i(u)$, which is obtained from the transverse integration of the reference heterogeneous equation (Eq. (8)), one is faced with the practical difficulty of obtaining

$\tilde{L}_i^{hom}(u)$ in order to solve the two-point boundary value problem. Fortunately, Koebke[5] recognised the fact that it is not as important to have the correct (exact) homogeneous transverse leakage shape as it is to use the same approximate transverse leakage distribution, both when solving the equivalent two-point boundary value problem (to obtain the $\hat{f}_i^{u\pm}$) and when solving the global homogenised reactor problem. Similarly, it is important to realise that any method, exact or approximate, can be used for the solution of the two-point boundary value problem to determine exact equivalence parameters, provided the same method is used in the global homogenised problem. This aspect of Koebke's ET, and of GET, is unique.

In most modern nodal methods, $\tilde{L}_i^{hom}(u)$ is approximated by means of a low-order polynomial expansion the coefficients of which are directly or easily obtained from the calculated nodal fluxes and currents. In fine-mesh finite difference (FMFD) methods (with multiple meshes per homogenised node) all coordinate directions are solved for simultaneously, and a transverse leakage term such as $\tilde{L}_i^{hom}(u)$ is therefore not directly used in such methods. For these methods it becomes difficult, if not impossible, to know what the transverse leakage shape will be when the homogenised problem is solved. In other words, the calculation of equivalent diffusion theory group constants for FMFD methods cannot in general be obtained directly from one-dimensional two-point boundary value problems, but requires an iteration between 1-D two-point boundary value problems and multi-dimensional, multi-node FMFD calculations of the global homogenised problem. In the so-called coarse-mesh finite difference method (CMFD) with one meshpoint in the centre of each homogenised node, a flat transverse leakage approximation is inherently made. Thus, GET (or ET) is easily applicable to the CMFD method.

5 THE ONE–DIMENSIONAL NGET METHOD

GET and ET can be incorporated into any nodal method which uses nodal surface averaged fluxes in the process of evaluating nodal coupling. In these methods the conventional continuity of interface average fluxes is replaced by the condition that $\hat{f}_i^{u+}\tilde{\phi}_i^{u+} = \hat{f}_{i+1}^{u-}\tilde{\phi}_{i+1}^{u-}$. It is easily shown that only the ratio, $\hat{f}_i^{u+}/\hat{f}_{i+1}^{u-}$, and not the actual values of the DF's, is of importance as far as nodal coupling is concerned. This fact forms the basis for the one–dimensional NGET method developed here.

We start by considering a one–dimensional (zero transverse leakage) system of homogenised slab nodes, for each of which the reference interface fluxes and net currents are known from a preceding calculation of the heterogeneous problem. The solution of the two–point boundary value problem for each node i then yields the $\hat{f}_i^{u\pm}$. Knowledge of these GET DF's allows one to calculate the ratios $\hat{f}_i^{u+}/\hat{f}_{i+1}^{u-}$ at each nodal interface of the global homogenised problem. One is then free to change the values of the GET DF's at any or all inner faces of the nodes, without affecting the net leakages across these interfaces or the nodal reaction rates and fluxes, provided the above ratios of DF's at the nodal interfaces are preserved.

In the NGET method as programmed in the code EQUIVA–1[8], we adjust all GET DF's to the right (+) of the left (–) interface of a given node i such that the right DF's of each node are set equal to its left (adjusted) DF's. In other words, for node i, we retain $\hat{f}_i^{u-}$ and set $\hat{f}_i^{u+}$ equal to $\hat{f}_i^{u-}$. For node i+1, we have to renormalise $\hat{f}_{i+1}^{u-}$ in order to maintain the original ratio $\hat{f}_i^{u+}/\hat{f}_{i+1}^{u-}$. Then $\hat{f}_{i+1}^{u+}$ is set equal to the renormalised value for $\hat{f}_{i+1}^{u-}$, etc. This renormalisation process then progresses through all the nodes up to the right boundary of the last node of the problem. In this way one obtains a single $\hat{f}_i$

for each node i. Obviously, the renormalisation procedure could be done in the reverse direction, or in both directions from an intermediate nodal interface.

Since these DF's are obtained by means of the normalisation of GET DF's, they are called Normalised GET (NGET) DF's and are henceforth indicated by $\hat{f}_i^{NGET}$. Having obtained a single $\hat{f}_i^{NGET}$ applicable to all faces of a node i (1–D in this case), it becomes possible to divide the FVW cross section and diffusion coefficient matrices of the node by this NGET DF matrix. By so doing, one derives an equivalent homogeneous diffusion equation system with continuity of interface fluxes.

This can also be achieved by means of the ET in 1–D (zero transverse leakage) since a single HF, $\hat{f}_i = \hat{f}_i^u$, is iteratively defined for each individual node, without any subsequent renormalisation as in the NGET method. In this case, the method is called the Simplified Equivalence Theory (SET) method by virtue of the fact that HF's do not appear explicitly in the equivalent diffusion equation[9]. It is important to note that in 1–D, the SET is exact. However, in practice, SET is also used for multi–dimensional nodes. In that case it is simply an approximation to ET in the sense that the HF's and diffusion coefficients in a specific coordinate direction are assumed to be valid in all directions.

In principle, the NGET method can similarly be applied to multi–dimensional problems by assuming a given coordinate direction to be representative of all other directions. However, this is generally a very unrealistic assumption since NGET is simultaneously applied to more than one node in the selected coordinate direction. The applicability of SET to realistic problems is much more general since it is applied to each node individually. Clearly, the two

methods are not identical. It is necessary to analyse both approaches in more detail to see the specific differences.

For simplicity, consider an equivalent homogenised problem consisting of only two slab nodes, i and i+1, with partial current albedo boundary conditions applied at the outer edges of the problem. For each node we know the reference interface net currents and fluxes, as well as the FVW cross sections and the GET DF's. For the present, it is assumed that the partial current albedo boundary conditions have been defined to conserve the reference net currents at the two boundaries of the problem. The definition of such a GET albedo boundary condition is discussed in the next section. For node i we then have

$$-\hat{D}_i \nabla_u^2 \tilde{\phi}_i(u) + \left[\hat{\Sigma}_{ti}^{hom} - \hat{\Sigma}_{si}^{hom} - \frac{1}{\lambda}\hat{F}_i^{hom}\right]\tilde{\phi}_i(u) = \tilde{0} \qquad (20)$$

and

$$-\hat{D}_i \nabla_u^2 \tilde{\phi}_i(u)\Big|_{u\pm} + \left[\hat{\Sigma}_{ti}^{hom} - \hat{\Sigma}_{si}^{hom} - \frac{1}{\lambda}\hat{F}_i^{hom}\right]\tilde{\phi}_i^{u\pm} = \tilde{0} \qquad (21)$$

where

$$-\hat{D}_i \nabla_u \tilde{\phi}_i(u)\Big|_{u\pm} = \tilde{J}_i^{u\pm} \qquad (22)$$

$$\tilde{\phi}_i^{u\pm} = \frac{1}{\hat{f}_i^{u\pm}}\,\tilde{\psi}_i^{u\pm} \qquad (23)$$

If, for node i, we assume

$$\hat{f}_i^{NGET} = \hat{f}_i^{u-} \quad , \qquad (24)$$

and replace $\hat{f}_i^{u+}$ by $\hat{f}_i^{NGET}$, then we also have to replace $\hat{f}_{i+1}^{u-}$ by

$$\hat{f}_{i+1}^{NGET} = \hat{f}_i^{NGET} \left[\frac{\hat{f}_{i+1}^{u-}}{\hat{f}_i^{u+}} \right] \tag{25}$$

to preserve the ratio of DF's at the common interface between nodes i and i+1. By now replacing $\hat{f}_{i+1}^{u+}$ by $\hat{f}_{i+1}^{NGET}$, we also obtain a single DF matrix for node i+1. However, this DF matrix will not conserve the reference net current, $\hat{J}_{i+1}^{u+}$, unless the original GET albedo boundary condition at this interface is also adjusted (renormalised) to reflect the replacement of $\hat{f}_{i+1}^{u+}$ by $\hat{f}_{i+1}^{NGET}$. For the present we assume this has been done; the calculation of the NGET albedo is discussed in the next section.

The solution of the global homogenised diffusion equation (coupled two–node problem) using the NGET DF's to compute nodal coupling, together with the NGET albedo's, will still preserve (directly or indirectly) all of the reference nodal quantities. We observe that the equivalent homogeneous diffusion equation, Eq. (20), can also be written as

$$-\hat{D}_i \frac{1}{\hat{f}_i^{NGET}} \nabla_u^2 \hat{f}_i^{NGET} \tilde{\hat{\phi}}_i(u) + \left[\hat{\Sigma}_{ti}^{hom} - \hat{\Sigma}_{si}^{hom} - \frac{1}{\lambda} \hat{F}_i^{hom} \right] \frac{1}{\hat{f}_i^{NGET}} \hat{f}_i^{NGET} \tilde{\hat{\phi}}_i(u) = \tilde{0} \, . \tag{26}$$

or equivalently as

$$-\hat{D}_i^{NGET} \nabla_u^2 \tilde{\hat{\phi}}_i^{NGET}(u) + \left[\hat{\Sigma}_{ti}^{NGET} - \hat{\Sigma}_{si}^{NGET} - \frac{1}{\lambda} \hat{F}_i^{NGET} \right] \tilde{\hat{\phi}}_i^{NGET}(u) = \tilde{0} \, . \tag{27}$$

A similar expression is obtained for node i+1. We further note that (see Eqs. (17) and (25))

$$\tilde{\phi}^{NGET}_{i+1}(u-) = \hat{f}^{NGET}_{i+1}\,\tilde{\phi}^{u-}_{i+1} = \frac{\hat{f}^{NGET}_{i+i}}{\hat{f}^{u-}_{i+1}}\,\tilde{\psi}^{u-}_{i+1}$$

$$= \frac{\hat{f}^{NGET}_{i}}{\hat{f}^{u+}_{i}}\,\tilde{\psi}^{u-}_{i+1} = \hat{f}^{NGET}_{i}\,\tilde{\phi}^{u+}_{i} = \tilde{\phi}^{NGET}_{i}(u+) \quad . \tag{28}$$

This expression shows that Eq. (27), in conjunction with conventional flux continuity conditions at nodal interfaces, defines an equivalent equation system for the homogenised global problem. For obvious reasons, the solution $\tilde{\phi}^{NGET}(u)$ to this global problem is called the NGET flux solution. This solution directly conserves all the required nodal quantities, with the exception of the node averaged flux. The node averaged flux can, however, be obtained indirectly:

$$\tilde{\Phi}^{av}_{i} = \tilde{\phi}^{av}_{i} = \frac{1}{V_i}\int_{V_i}\tilde{\phi}_i(r)dr = \frac{1}{h_i}\int_{h_i}\tilde{\phi}_i(u)du$$

$$= \frac{1}{\hat{f}^{NGET}_{i}}\,\frac{1}{h_i}\int_{h_i}\tilde{\phi}^{NGET}_{i}(u)du = \frac{1}{\hat{f}^{NGET}_{i}}\,\frac{1}{V_i}\int_{V_i}\tilde{\phi}^{NGET}_{i}(r)dr \quad . \tag{29}$$

A similar expression must be used to recover the node averaged fluxes from a SET solution. In SET one also has continuity of the SET flux solution:

$$\tilde{\phi}^{SET}_{i}(u+) = \hat{f}^{SET}_{i}\,\tilde{\phi}^{u+}_{i} = \hat{f}^{SET}_{i+1}\,\tilde{\phi}^{u-}_{i+1} = \tilde{\phi}^{SET}_{i+1}(u-) \quad . \tag{30}$$

Moreover, since $\hat{f}_i^{SET} = \hat{f}_i^{u}$, one has that (Eq. (23))

$$\tilde{\phi}_i^{SET}(u+) = \tilde{\psi}_i^{u+} = \tilde{\psi}_{i+1}^{u-} = \tilde{\phi}_{i+1}^{SET}(u-) \quad . \tag{31}$$

Thus, the SET interface averaged fluxes are equal to the physically continuous heterogeneous interface averaged fluxes. In multi-dimensional applications this is only approximately true (because SET is an approximation to ET). In contrast, the NGET interface fluxes, although continuous, are not equal to the physical interface averaged fluxes. There is, of course, one exception, namely at the left (-) interface of node i. For this node the NGET DF's are equal to the GET DF's at this face.

This illustrates an important difference between NGET and SET. If the physical interface averaged fluxes are needed for some purpose, then NGET requires additional algebra, as well as knowledge of both the NGET and the original GET DF's, to obtain them:

$$\tilde{\psi}_{i+1}^{u-} = \tilde{\psi}_i^{u+} = \frac{\hat{f}_i^{u+}}{\hat{f}_i^{NGET}} \tilde{\phi}_i^{NGET}(u+) = \frac{\hat{f}_{i+1}^{u-}}{\hat{f}_{i+1}^{NGET}} \tilde{\phi}_{i+1}^{NGET}(u-) \quad . \tag{32}$$

As far as the ex-core regions of a PWR are concerned, we do not demand knowledge of reaction rates or fluxes within these regions. As a result, the above-mentioned complexities of the NGET are not relevant. It should be emphasised here that the NGET is intended primarily for application to the ex-core nodes of a PWR, while GET or ET may be applied to the core region. Hence, node i is defined as the first ex-core node adjacent to the core fuel nodes (i.e. $\hat{f}_i^{NGET} = \hat{f}_i^{u-}$). Other possible applications of NGET are discussed in Section 9.

6 EQUIVALENT ALBEDO BOUNDARY CONDITIONS

In the previous section we assumed that partial current albedos, which are consistent with either the GET or the NGET parameters, had been defined to conserve the face averaged net currents on the outer faces of the global homogenised problem. We shall first discuss the definition of a diagonal GET partial current albedo boundary condition matrix

$$\tilde{\tilde{J}}^{(in)u+}_{i+1} = \hat{A}^{u+}_{i+1}\ \tilde{\tilde{J}}^{(out)u+}_{i+1} \qquad (33)$$

We make use of the conventional diffusion theory definition of partial currents:

$$\begin{aligned} \tilde{\tilde{J}}^{(in)u+}_{i+1} &= \tfrac{1}{4}\ \hat{f}^{+}_{i+1}\tilde{\tilde{\phi}}^{u+}_{i+1} + \tfrac{1}{2}\ \hat{D}_{i+1}\ \nabla_u \tilde{\tilde{\phi}}_{i+1}(u)\big|_{u+} \quad ; \\ \tilde{\tilde{J}}^{(out)u+}_{i+1} &= \tfrac{1}{4}\ \hat{f}^{+}_{i+1}\tilde{\tilde{\phi}}^{u+}_{i+1} - \tfrac{1}{2}\ \hat{D}_{i+1}\ \nabla_u \tilde{\tilde{\phi}}_{i+1}(u)\big|_{u+} \end{aligned} \qquad (34)$$

Clearly,

$$\tilde{\tilde{J}}^{u+}_{i+1} = \tilde{\tilde{J}}^{(out)u+}_{i+1} - \tilde{\tilde{J}}^{(in)u+}_{i+1} \qquad (35)$$

Substitution of Eq. (34) in Eq. (33), and making use of Eqs. (22) and (23), yields

$$\langle G|A^{u+}_{i+1}|G\rangle = \frac{\langle G|\psi^{u+}_{i+1}\rangle - 2\langle G|J^{u+}_{i+1}\rangle}{\langle G|\psi^{u+}_{i+1}\rangle + 2\langle G|J^{u+}_{i+1}\rangle} \qquad (36)$$

A similar expression can be obtained for $\langle G|A^{u-}_{i}|G\rangle$. The use of this GET albedo is necessary to define an equivalent homogenised problem. Note that for $\tilde{J}^{u+} = \tilde{0}$, $\hat{A}^{u+} = E$, and the GET DF's do not play a role in the definition

of the albedo. This is consistent with the fact that the ratio of the GET DF's is unity for zero net currents at an interface.

The ET requires a corresponding ET albedo matrix (simply replacing $\hat{f}^{u+}_{i+i}$ by $\hat{f}^{u}_{i+1}$ in Eq. (34)) to define an equivalent homogenised problem.

No reference has been found in the open literature with regard to the definition of such equivalent boundary conditions. This is probably due to the fact that in most modern nodal methods in which the GET or ET is used, boundary conditions are applied only on the outer edge of the reflector. Since the reflector nodes are usually sufficiently thick to make the transmission probability of these nodes very small, the need for equivalent boundary conditions may not have been emphasised in the literature. A more likely reason for this may be the fact that transverse integration nodal methods cannot accurately utilise boundary conditions by virtue of the fact that the transverse leakage approximation is generally based on information which is excluded by the boundary conditions. It may then be argued that an exact equivalent partial current albedo boundary condition matrix (or any other equivalent boundary condition) is of little use if it leads to other inaccuracies.

Our reason for including the above definition in the discussion is directly related to the fact that we also use the NGET parameters for PWR ex-core nodes in codes which do not necessarily make assumptions regarding transverse leakages and therefore treat albedo boundary conditions exactly (within the framework of diffusion theory). The diagonal NGET partial current albedo matrix differs from the GET matrix by virtue of the normalisation of the GET DF's to obtain the NGET parameters.

If the coefficients in the diffusion equation are the NGET cross sections and diffusion coefficients, then partial currents are defined as in Eq. (34), but with NGET parameters:

$$\tilde{\tilde{J}}^{(in)NGET}_{i+1}(u+) = \frac{1}{4}\tilde{\tilde{\phi}}^{NGET}_{i+1}(u+) + \frac{1}{2}\hat{D}^{NGET}_{i+1}\nabla_u\tilde{\tilde{\phi}}^{NGET}_{i+1}(u)\Big|_{u+} ;$$

$$\tilde{\tilde{J}}^{(out)NGET}_{i+1}(u+) = \frac{1}{4}\tilde{\tilde{\phi}}^{NGET}_{i+1}(u+) - \frac{1}{2}\hat{D}^{NGET}_{i+1}\nabla_u\tilde{\tilde{\phi}}^{NGET}_{i+1}(u)\Big|_{u+} . \quad (37)$$

Recalling that

$$-\hat{D}^{NGET}_{i+1}\nabla_u\tilde{\tilde{\phi}}^{NGET}_{i+1}(u)\Big|_{u+} = \tilde{\tilde{J}}^{u+}_{i+1} , \quad (38)$$

and

$$\tilde{\tilde{\phi}}^{NGET}_{i+1} = \frac{\hat{f}^{NGET}_{i+1}}{\hat{t}^{u+}_{i+1}}\tilde{\tilde{\psi}}^{u+}_{i+1} \quad (39)$$

we find

$$\langle G|A^{NGET}_{i+1}(u+)|G\rangle$$

$$= \frac{\langle G|f^{NGET}_{i+1}|G\rangle\langle G|\psi^{u+}_{i+1}\rangle - 2\langle G|f^{u+}_{i+1}|G\rangle\langle G|J^{u+}_{i+1}\rangle}{\langle G|f^{NGET}_{i+1}|G\rangle\langle G|\psi^{u+}_{i+1}\rangle + 2\langle G|f^{u+}_{i+1}|G\rangle\langle G|J^{u+}_{i+1}\rangle} . \quad (40)$$

This is the **diagonal NGET** partial current albedo boundary condition matrix which conserves the surface averaged reference net group currents at a nodal interface.

It should be noted that the elements of the NGET as well as the GET partial current albedo matrices can take on unphysical negative (real) values.

7 ANALYTIC SOLUTION TO THE TWO-POINT BOUNDARY VALUE PROBLEM

One of the objectives of this work is to define an equivalent PWR reflector model which is applicable to conventional fine-mesh finite difference methods (mesh-centred and mesh-cornered) as well as to advanced nodal methods. This compatability is achievable only in the case of the analytic nodal method, or at least in cases where the ex-core nodes are treated analytically by the nodal method. This is one of the reasons why we have chosen to calculate the NGET cross sections by means of a few-group (not limited to two groups) analytic diffusion theory solution to the two-point boundary value problem.

The analytic solution to the few-group diffusion equation for a given homogenised node requires the calculation of functions of matrices. This has traditionally presented numerical problems which have recently been overcome[12] by using similarity transformations to diagonalise the problematic matrix functions. The details of this basis transformation procedure and the analytic solution to the 1-D few-group diffusion equation for a homogeneous medium are presented in Appendix A. Here it suffices to simply give the final few-group analytic diffusion theory flux solution within a homogenised node. In the dimensionless local coordinate system of the node, this solution is given by Eq. (A.15):

$$\underset{\sim}{\phi}(\xi) = \frac{\sin \hat{B}(1-\xi)}{\sin 2\hat{B}} \underset{\sim}{\phi}^{-} + \frac{\sin \hat{B}(1+\xi)}{\sin 2\hat{B}} \underset{\sim}{\phi}^{+} \quad . \tag{41}$$

This is not the actual result we seek to determine the GET discontinuity factors on the faces of the node. For this purpose we require the values of the homcgeneous flux distribution at the node edges. One way of obtaining the boundary fluxes is based on the T–response matrix[12,23] relationship, which is derived in Appendix B. This relationship states:

$$\tilde{\underline{\phi}}_n = \hat{\underline{\underline{T}}}\, \tilde{\underline{\phi}} \quad , \tag{42}$$

where $\hat{\underline{\underline{T}}}$ is a 2Kx2K matrix which is directly calculable from the K–group FVW cross section data of the node. It relates the normal outgoing gradients of the flux on the two node boundaries to the flux values at these points. By direct inversion of this matrix one then obtains the required boundary fluxes in terms of the known reference outgoing boundary currents (see Eqs. (A.4), (B.10), (B.11)):

$$\tilde{\underline{\phi}} = \hat{\underline{\underline{T}}}^{-1}\, \tilde{\underline{\phi}}_n = \frac{-h}{2}\, \hat{\underline{\underline{T}}}^{-1}\, \hat{\underline{\underline{D}}}^{-1}\, \tilde{\underline{J}}_n \quad . \tag{43}$$

The procedure for calculating the T–response matrix and thereby the node interface fluxes according to Eq. (43), has been programmed in the code EQUIVA–1[8].

A more economical means of obtaining the homogeneous interface fluxes would be to calculate the elements of the $\hat{T}^{-1}$–response matrix[12,23] directly, without first calculating $\hat{T}$ and then inverting it. The direct calculation of $\hat{T}^{-1}$ from the FVW cross section data of the node is discussed in Appendix C. This approach has not been included in EQUIVA–1. However, a second approach, based on the R–response matrix[12,23] formalism, has also been included in EQUIVA–1. The expression used to determine the homogeneous interface fluxes from the

R–response matrix calculated from the FVW cross section of a given homogenised node is

$$\tilde{\underline{\phi}} = -2(\hat{\underline{\underline{E}}} + \hat{\underline{\underline{R}}})(\hat{\underline{\underline{E}}} - \hat{\underline{\underline{R}}})^{-1}\, \tilde{\underline{J}}_n \quad . \tag{44}$$

This expression is obtained by substitution in Eq. (43) of the relationship (D.6) between the R and T matrices. The calculation of the R–response matrix from the diffusion theory group constants of a given homogeneous node is detailed in Appendix D.

The homogeneous boundary fluxes calculated according to either Eq. (43) or Eq. (44) can take on negative values. Consequently, negative DF's can be calculated by means of Eq. (18) and hence negative NGET cross sections may be obtained. To ensure convergence of the flux solution in nodal codes, it is therefore required that DF's be positive. A natural requirement to ensure this is to demand that the homogeneous flux be non–negative and finite everywhere. For a multiplying node with $\lambda < k_\infty$, this implies that the real fundamental mode eigenvalue $\left[b_1^2\right]$ of the buckling matrix must be positive and smaller than $\left[\frac{\pi}{2}\right]^2$. This follows from the fact that the finiteness of $<\beta_1|\phi(\xi)>$ implies that $\sin 2b_1 \neq 0$, while the positivity of

$$<\beta_1|\phi(0)> = \frac{1}{\cos\, b_1}\,(<\beta_1|\phi^->\, + <\beta_1|\phi^+>) \tag{45}$$

implies that $|b_1| < \frac{\pi}{2}$. This test has heen included in the code EQUIVA–1 in the form of $b_1^2 < \left[\frac{\pi}{2}\right]^2$. Note that this test is based on the assumption that the sum of the face averaged fundamental mode fluxes is positive. It does not therefore guarantee positive fluxes everywhere, but merely expresses the fact that if the fundamental mode buckling b_1^2 is not smaller than $\left[\frac{\pi}{2}\right]^2$, then such a guarantee does not exist.

For multiplying nodes with $\lambda > k_\infty$ and for non–multiplying nodes, the above test is meaningless since the fundamental mode eigenvalue $\left[b_1^2\right]$ is negative and hence the fundamental mode flux distribution is described by hyperbolic functions.

In an attempt to detect possible negative flux values within a homogeneous node, EQUIVA–1 includes a simple test for possitivity of the few–group interface and node midpoint fluxes. In the case where negative fluxes are detected, use is made of the fact that the diffusion coefficient matrices are arbitrary and that the solution to the 2–point boundary value problem is strongly coupled to these diffusion coefficients. In EQUIVA–1, the diffusion coefficient matrices are then multiplied by an arbitrary constant until the solution to the 2–point boundary value problem yields positive interface and midpoint fluxes. This constant is chosen to be greater than unity. The reasoning behind this choice is as follows:

The solution to the 2–point boundary value problem conserves the reference interface leakages as well as the positive node average flux. Thus, if this solution yields negative interface fluxes at either one or both of the node faces, then the homogeneous flux solution must have rather steep gradients at the node faces. In order to reduce the steepness of these gradients while preserving the reference interface currents, the diffusion coefficients must be increased. In the case of negative midpoint fluxes, the inherent problem is also steep flux gradients, and increasing the value of $\hat{D}$ is also a valid procedure for this case. In practice, negative interface fluxes for homogenised PWR baffle/reflector nodes are frequently calculated from conventional FVW cross sections. The above adjustment procedure has been found to be successful in all cases encountered thus far.

A test which has proved to be extremely useful for detecting input data errors to the code EQUIVA–1 is that of comparing the input reference node averaged fluxes with the node averaged fluxes calculated according to Eq. (C.4).

8 SUMMARY OF THE ADVANTAGES OF THE NGET METHOD FOR PWR REFLECTOR MODELLING

Before considering the possible benefits or advantages of the NGET with respect to the modelling of the ex–core regions of a PWR, one has to note that in practice a reference reactor solution is not available for the generation of equivalent cross sections. The usual practice is therefore to assume that solutions to very simple heterogeneous problems which appropriately simulate spectral conditions in parts of the reactor can be taken as references for generating equivalent parameters. In the case of the ex–core regions of a PWR, a simple slab model of a part of the core and the ex–core nodes is adequate[3,4].

As pointed out previously, we are primarily interested in modelling core leakages accurately and are not interested in the actual values of fluxes or reaction rates within the ex–core regions. The use of NGET cross sections achieves this goal without undue complications to nodal cross section library structures and data handling facilities. Since flux discontinuities are directly included in the NGET cross sections for the ex–core nodes, the same number of homogenisation parameters as in conventional FVW is used per node. Thus, conventional library representations can be used for the NGET cross sections. The same can be said for SET. In contrast, GET and ET introduce additional homogenisation parameters that need to be included in cross section libraries and as a result also complicate data handling.

In comparison with SET, the NGET method has the advantage that the calculation of equivalent parameters for the ex–core nodes is simplified since an iterative procedure is not required to obtain these parameters.

The limitations of the NGET should also be mentioned. Firstly, the NGET is easily applicable only to 1–D slab geometries. This is not the case with SET and it (SET) is therefore also widely used for 2–D PWR assembly homogenisation. Secondly, the NGET method is simultaneously applied to a number (set) of nodes. This inherently implies that the NGET cross sections of a given node are dependent on the heterogeneities and spectral details within other nodes of the set. This sensitivity, which may be quite severe, is not inherent in the SET (or ET and GET). However, as far as the ex–core nodes of a PWR are concerned, this is not an actual disadvantage since the ex–core nodes occur in exactly the geometrical order in which they are modelled in the heterogeneous spectral calculation. Moreover, the GET DF's on the inner face of the first ex–core node adjacent to the core are retained. This is a common feature to all PWR reflector models based on the ET or GET[3,10,13].

In conclusion, it can be stated that the NGET method has no disadvantages relative to the other mentioned methods with regard to the 1–D modelling of the ex–core nodes of a PWR, but in fact may be considered to have certain practical advantages. The equivalent albedo boundary conditions formulated in this report have also been found useful when PWR ex–core nodes of one quarter the size of an assembly (radially) are used in reactor calculations[4].

9 OTHER PRACTICAL APPLICATIONS OF NGET

The 1–D NGET method can clearly be applied to coarse–mesh finite difference (CMFD) problems in slab geometry. In such applications one meshpoint in the

centre of each homogenised node is considered and DF's are defined to conserve the reference face averaged currents and node averaged reaction rates. The form of the CMFD net leakage term permits the direct calculation of the GET as well as the NGET DF's from the reference nodal parameters, without the need for the numerical solution of a two–point boundary value problem. To illustrate this, let us consider again the two–node slab problem of Section 8.

In the CMFD we include GET DF's in the gradient term such that the reference face averaged normal outgoing currents and the node averaged fluxes are conserved:

$$<G|J^{u+}_{n\,i}> = \frac{-2<G|D_i|G>}{h_i}\left[\frac{<G|\psi^{u+}_i>}{<G|f^{u+}_i|G>} - <G|\phi^{av}_i>\right]$$

$$= - <G|J^{u-}_{n,i+1}> = \frac{2<G|D_{i+1}|G>}{h_{i+1}}\left[\frac{<G|\psi^{u-}_{i+1}>}{<G|f^{u-}_{i+1}|G>} - <G|\phi^{av}_{i+1}>\right] \qquad (46)$$

The GET DF's at the interface between nodes i and i+1 are then calculated according to

$$<G|f^{u+}_i|G> = \frac{2<G|D_i|G><G|\psi^{u+}_i>}{2<G|D_i|G><G|\phi^{av}_i> - h_i<G|J^{u+}_{n\,i}>} \quad , \qquad (47)$$

$$<G|f^{u-}_{i+1}|G> = \frac{2<G|D_{i+1}|G><G|\psi^{u-}_{i+1}>}{2<G|D_{i+1}|G><G|\phi^{av}_{i+1}> - h_{i+1}<G|J^{u-}_{n,i+1}>} \quad . \qquad (48)$$

By now renormalising DF's according to Eq. (25), one defines NGET DF's and NGET cross sections which yield the conventional mesh–centred finite difference

expressions for nodal coupling. The expressions for the equivalent albedo boundary conditions in Section 6 are also directly applicable to the finite difference problem since the DF's automatically account for the finite difference approximation.

This approach can be used in practical diffusion theory assembly depletion calculations in which equivalent cross sections for inter-assembly water gaps, control blades and burnable poison curtains are required. Geometrically simple slab supercell transport theory calculations are generally used as references for generating equivalent cross sections for such regions. A typical supercell which would be used for this purpose usually consists of a central heterogeneous absorber cell and several adjacent fuel cells, with the problem having central symmetry. The left and right GET DF's for the homogenised central cell (node i) are then identical. NGET DF's for this node can be calculated as the ratio

$$\langle G|f_i^{NGET}|G\rangle = \frac{\langle G|f_i^{u+}|G\rangle}{\langle G|f_{i+1}^{u-}|G\rangle} \tag{49}$$

$$= \left[\frac{2\langle G|D_{i+1}|G\rangle\langle G|\phi_{i+1}^{av}\rangle - h_{i+1}\langle G|J_{n,i+1}^{u-}\rangle}{2\langle G|D_i|G\rangle\langle G|\phi_i^{av}\rangle - h_i\langle G|J_{ni}^{u+}\rangle}\right]\frac{\langle G|D_i|G\rangle}{\langle G|D_{i+1}|G\rangle},$$

while the NGET DF's for node i+1 are taken as unity. As a matter of practical convenience one can then assume that the NGET DF's for all the nodes other than the central absorber node are unity. This approximate NGET method has been coded in EQUIVA-1[8] and is used to generate equivalent NGET cross sections for strong slab absorbers and inter-assembly water gaps. These NGET cross sections are used in typical assembly depletion calculations with 1 meshpoint per homogenised cell. It is of some interest to note that this particular application does not involve the assumption that nodes i and i+1 have

the same size (width). This has the practical benefit that inter-assembly and intra-assembly mesh sizes need not be identical.

A similar application of the NGET to 2-D supercell problems is possible. Typical supercells consist of a 3x3 matrix of eight fuel cells surrounding a central heterogeneous absorber cell, with the problem having octant symmetry. The approximate application of NGET to this problem would again involve calculating only the NGET DF matrix for the central homogenised cell according to Eq. (49). It should be noted that in this particular application the nodes all have the same size (i.e. $h_i = h_{i+1} = h$). In practice, the 2-D supercell is often approximated by a 1-D cylindrical supercell consisting of two concentric rings of homogenised fuel, each representing four fuel cells, surrounding the central heterogeneous absorber cell. Since only the total net leakages across the concentric nodal interfaces are known from such a calculation, one has to recast Eq. (49) into a form which contains only total net leakages from the central node. This is easily done by observing that the total leakage from node i is given by

$$\tilde{L}_{ni}^{tot} = 4S_i\tilde{J}_{ni}$$

Using this, together with the fact that $S_i = h_i = h$ for this problem, reduces Eq. (49) to

$$\langle G|f_i^{NGET}|G\rangle = \frac{\langle G|f_i^{u+}|G\rangle}{\langle G|f_{i+1}^{u-}|G\rangle} \tag{50}$$

$$= \left[\frac{8\langle G|D_{i+1}|G\rangle\langle G|\phi_{i+1}^{av}\rangle - \left[-\langle G|L_{ni}^{tot}\rangle\right]}{8\langle G|D_i|G\rangle\langle G|\phi_i^{av}\rangle - \langle G|L_{ni}^{tot}\rangle}\right]\frac{\langle G|D_i|G\rangle}{\langle G|D_{i+1}|G\rangle}$$

This expression has also been coded in EQUIVA-1 for the purpose of generating equivalent cross sections for PWR control rods, burnable absorber rods, or guide thimbles. These cross sections can be used in conjunction with conventional FVW fuel cell cross sections in 2-D assembly depletion calculations by means of a conventional mesh-centred finite difference diffusion code with one mesh per homogenised cell.

It is important to note that the GET DF's calculated according to Eqs. (47) and (48) can be negative. To avoid this, the diffusion coefficients for a given node i must be adjusted such that

$$<G|D_i|G> \; > \frac{h_i}{2<G|\phi_i^{av}>} \max\left[<G|J_{n\,i}^{u+}> \;,\; <G|J_{n\,i}^{u+}>\right] \quad . \tag{51}$$

In slab geometry this test is easily performed for each node. In 2-D geometry the test must be done for both coordinate directions. In the case of a 1-D cylindrical supercell, this expression cannot be applied directly to each node, and attention should rather be fixed on defining a positive NGET DF matrix for the central node. From Eq. (50) the following requirements are obtained:

$$\begin{aligned} <G|D_i|G> \; &> \frac{1}{8<G|\phi_i^{av}>}<G|L_{ni}> \quad , \\ <G|D_{i+1}|G> \; &> \frac{-1}{8<G|\phi_{i+1}^{av}>}<G|L_{ni}> \quad . \end{aligned} \tag{52}$$

Other applications of the NGET may be possible. Here we have presented only the simplest and most obvious ones. These specific applications are currently used on a routine basis for generating equivalent cell cross sections for the strong absorbers and water gaps which are present in light-water reactor fuel

assemblies. The approximate NGET method presented here is similar to the "rodded cell adjustment" procedure described by Tanker and Henry[14] for strong absorber cells. It also has some connection with the DMOD method used in the LWR–WIMS assembly depletion code[15]. If the NGET DF in Eq. (49) is set to unity and one solves for $\hat{D}_i$, the DMOD approximation is obtained. Despite this apparent equivalence, the DMOD method has the disadvantage that negative diffusion coefficients may be calculated for node i.

10 PRACTICAL CALCULATION OF FVW DIFFUSION COEFFICIENTS

As far as the calculation of DF's is concerned, the definition of diffusion coefficients is quite arbitrary. However, there are two practical considerations which should be taken into account when calculating the $\hat{D}$'s. The first is the fact that the $\hat{D}$ for a given node must often be constructed from microscopic cross sections and consequently a specific recipe for calculating the $\hat{D}$ may be required. The other is related to the fact that, depending on the definition of the $\hat{D}$, conventional FVW cross sections are often adequate for some nodes and DF's need not be determined. This is for instance the case for homogenised PWR assemblies[3]. It is thus of some interest, even if only to be consistent, to establish a practical procedure for calculating $\hat{D}$'s.

In those cases where DF's are not calculated for homogenised nodes, it is preferable to give some theoretical basis to the definition of the FVW diffusion coefficients. The P_1 equations provide the most natural choice for such a theoretical basis. These equations are[16]:

$$\nabla\cdot\tilde{J} + \hat{\Sigma}_t\tilde{\psi} = \hat{\Sigma}_{s0}\tilde{\psi} + \frac{1}{\lambda}\hat{F}\tilde{\psi} \quad ,$$

$$\nabla\tilde{\psi} + 3\hat{\Sigma}_{t1}\tilde{J} = 3\hat{\Sigma}_{s1}\tilde{J} \quad . \tag{53}$$

Here $\hat{\Sigma}_{t1}$ is the current-weighted total cross section matrix and $\hat{\Sigma}_{s1}$ is the current-weighted P_1 scattering matrix. The second equation is used to define the diffusion coefficient matrix:

$$\hat{D} = \frac{1}{3}\left[\hat{\Sigma}_{t1} - \hat{\Sigma}_{s1}\right]^{-1} = \frac{1}{3}\hat{\Sigma}_{tr}^{-1} \quad . \tag{54}$$

In practice, various approximations are employed to diagonalise the diffusion coefficient matrix. These approximations will not be discussed here. What is of importance here, is the approximations that are made in homogenising and collapsing the P_1 equations to define few-group diffusion coefficient matrices such that their use in the diffusion equation will yield the best results when conventional FVW is used for the other cross section matrices in the diffusion equation (the P_0 equation).

According to Eq. (54), the $\hat{D}$ is calculated from a macroscopic transport matrix. The transport matrix itself is calculated from the number densities and microscopic transport matrices of the individual elements (or isotopes) that constitute the material region in which the P_1 equations are defined:

$$\hat{\Sigma}_{tr} = \sum_j N^j \hat{\sigma}_{tr}^j \quad . \tag{55}$$

This expression can also be interpreted as the mixing of the inverse of the microscopic diffusion coefficient matrices calculated from the individual microscopic transport cross sections. This equation forms the basis for the rest of the discussion.

As far as homogenisation is concerned, one considers the P_1 equations integrated over the combined volumes of several continuous material regions. FVW cross sections can then be defined and used in the first equation of Eq. (53), and

current–volume weighted (CVW) cross sections in the second equation. This does not define an equivalent P_1 equation system for the homogenised problem since no attempt has been made to preserve interface leakages. In other words, the $\hat{D}$ calculated from the CVW cross sections according to Eq. (54) does not enable an equivalent diffusion problem to be defined. One may then argue that the CVW cross section used in the second of the two P_1 equations might as well be replaced by their FVW values. This is usually done in practice. Either way, the most important point here is that both averaging methods determine that microscopic transport cross sections, and not their inverses, must be homogenised to maintain consistency with Eq. (55). Note that the volume averaged number densities of the constituents should be used in Eq. (55).

From the above it is clear that microscopic transport cross sections should be mixed and homogenised if the P_1 equations are taken as basis for determining diffusion coefficients. However, it can be shown that if arbitrary microscopic diffusion coefficients are used, then consistency is also obtained if the microscopic diffusion coefficients are mixed and homogenised. A combination of transport mixing and microscopic diffusion coefficient homogenisation (or vice versa) is not consistent.

With regard to the group collapsing of the P_1 equations, they show that microscopic transport matrices should be current–collapsed to ensure consistency with current–collapsed macroscopic transport matrices. This seems simple enough, but there are some practical problems with this approach.

Firstly, currents can vary in sign from group to group and as a result a true "averaging" procedure is not followed. Taking the absolute values of the currents may be considered as an acceptable solution to this problem. Secondly, many spectrum codes do not calculate currents and hence use only scalar fluxes

for group collapsing. This obstacle is easily overcome by assuming, in addition to Fick's law for the current, that the scalar flux is separable in space and energy. This leads to a definition for the flux collapsing of the inverse of the macroscopic transport matrix in order to obtain the few–group diffusion coefficient matrix. Similar collapsing of the inverse microscopic transport matrices does not satisfy Eq. (55). This inconsistency was first noted by Zweifel and Ball[17]. Travelli[18] devised a definition for few–group microscopic transport matrices which satisfy Eq. (55) with flux–collapsed inverse macroscopic transport matrices. Travelli's definition also satisfies the practically necessary condition that

$$\frac{\partial \hat{\Sigma}_{tr}}{\partial N^j} = \hat{\sigma}^j_{tr} \quad . \tag{56}$$

The only assumption that Travelli makes is that, within each broad–group, the change in the collision density due to a small composition change does not depend on the energy. Travelli's definition for the few–group microscopic transport matrices is recommended if scalar fluxes are used as weighting functions. The order in which mixing, homogenisation, and group collapsing takes place is not important if Travelli's assumption regarding the change in the collision density is adequate. If only macroscopic homogenised cross sections are collapsed, it is recommended that the $\hat{D}$'s and not the $\hat{\Sigma}_{tr}$'s be flux–collapsed.

As far as the GET or the NGET is concerned, it is recommended that FVW diffusion coefficient matrices calculated according to the above procedure be used in the solution of the two–point boundary value problem. It should be pointed out that the division of the FVW macroscopic $\hat{D}$'s by the NGET DF's implies the multiplication of the FVW microscopic transport matrices by the NGET DF's.

11 CONCLUDING REMARKS

The NGET method developed in this report for the modelling of the ex–core regions of a PWR yields equivalent cross sections for these regions which can be used in conventional fine–mesh finite difference and advanced transverse integration nodal diffusion codes. In the case of the advanced nodal codes, an analytic diffusion method should be used in the ex–core nodes. The calculation of NGET cross sections for the ex–core nodes for use with another nodal approximation such as, for example, the Nodal Expansion Method (NEM), simply requires that the two–point boundary value problem be solved by this method rather than the analytic method developed in this work.

The application of the NGET method to assembly spectrum calculations by means of conventional mesh–centred finite difference diffusion codes has also been addressed. A prescription for calculating NGET cross sections for strong absorbers and thermal flux traps (water gaps) by means of simple supercell calculations was presented. These equivalent cross sections are expected to perform as well in assembly spectrum calculations as other types of equivalent cross sections derived from such supercell calculations. (Some of the more popular methods used to define such equivalent cross sections are mentioned in Reference 19.)

A novel idea introduced in this report is that of the calculation of equivalent partial current albedo boundary conditions to ensure that an equivalent homogeneous diffusion equation system is indeed defined. Although this idea is inherently implied by the Equivalence Theory, an explicit formula for the calculation of equivalent boundary conditions has not been found in the open literature. Such a formula is given in Section 6 of this report. The NGET albedo boundary conditions have been used in 2–D PWR calculations and it has

been successfully demonstrated that they are essential for accurate PWR analyses if only a small part of the radial ex–core regions is explicitly modelled[4]. However, these calculations were done with methods that are not based on the transverse integration procedure. Therefore, the utility of equivalent boundary conditions used in conjunction with transverse integration nodal methods remains a controversial subject.

In conclusion, it can be stated that the NGET method is very successful for the modelling of the ex–core regions of a PWR. It is expected to be similarly successful in fuel assembly spectrum analyses (cell homogenisation), but this has not been satisfactorily demonstrated. Future development of the NGET method would seem to be restricted to improving the flexibility of the NGET cross sections for the homogenised baffle/reflector nodes of a PWR with respect to changing core conditions. The numerical results presented in Reference 4 suggest that such an improvement can be justified, if it is based on a straightforward extension of the procedure presently used.

12 REFERENCES

[1] KOEBKE K, et al.: "Principles and Applications of Advanced Nodal Reactor Analysis Methods". Atomkernenergie 46, 221 (1985).

[2] SMITH K S: "Advanced Nodal Diffusion Methods". Lecture 3 of "Modern Nodal Methods for Analyzing Light Water Reactors", MIT Special Summer Session, June 23–27, 1986.

[3] SMITH K S: "Assembly Homogenisation Techniques for Light Water Reactor Analysis". Prog. Nucl. Energy 17, 303 (1986).

[4] MÜLLER E Z: "Validation of the One–Dimensional NGET Homogenised Baffle/Reflector Model". Internal Report RTE01–2/2–031 of the Reactor Theory Division, Atomic Energy Corporation of South Africa, (1987).

[5] KOEBKE K: "A New Approach to Homogenization and Group Condensation". IAEA Technical Committee Meeting on Homogenization Methods in Reactor Physics, Lugano, Switzerland, Nov. 13–15, 1978. IAEA–TECDOC–231 (1980).

[6] SMITH K S: "Spatial Homogenization Methods for Light Water Reactor Analysis". Ph.D. Thesis, Dept. Nucl. Eng., MIT, 1980.

[7] MÜLLER E Z: "A Brief Introduction to the Dirac Bra–Ket Notation for use in Nodal Methods". Internal Report RTE01–2/2–056 of the Reactor Theory Division, Atomic Energy Corporation of South Africa (1989).

[8] MÜLLER E Z: "EQUIVA–1: A Code for Generating One–Dimensional NGET Cross Sections for PWR Ex–Core Regions". Report PEL 301, (1991).

[9] KOEBKE K: "Advances in Homogenization and Dehomogenization". ANS/ENS Int. Top. Meet. on Advances in Mathematical Methods for the Solution of Nuclear Engineering Problems, München, FRG, Apr. 27–29, 1981.

[10] KOEBKE K, et al.: "Application and Verification of the Simplified Equivalence Theory for Burnup States". Nucl. Sci. Eng. 92, 56 (1986).

[11] BONALUMI R A: "Rigorous Homogenized Diffusion Theory Parameters for Neutrons". Nucl. Sci. Eng. 77, 219 (1981).

[12] WEISS Z J: "Lecture Notes on Nodal Methods". Lectures presented at Pelindaba during 1984–1985.

[13] RATHKOPF J A and LIU Y S: "A Method of Baffle/Reflector Region Homogenization". Trans. Am. Nucl. Soc. 53, 247 (1986).

[14] TANKER E and HENRY A F: "Finite Difference Group–Diffusion Theory Parameters that Reproduce Reference Results". Trans. Am. Nucl. Soc. 50, 280 (1985).

[15] HALSALL M J: "LWR–WIMS, A Computer Code for Light Water Reactor Lattice Calculations". Report AEEW–R 1498 (1982).

[16] HENRY A F: "Nuclear–Reactor Analysis", MIT Press, 1975.

[17] ZWEIFEL P F and BALL G L: "Group Cross–Sections for Fast Reactors". Proc. Seminar on the Physics of Fast and Intermediate Reactors, Paper SM–18/65, Vol II, IAEA, Vienna, 1962.

[18] TRAVELLI A: "A New Definition of the Microscopic Multigroup Transport Cross Sections". Trans. Am. Nucl. Soc. 11, 532 (1968).

[19] MÜLLER E Z: "A Review of Some Cross Section Generation Methodologies for Nodal Analysis of Pressurized Water Reactors". Internal Report RTE01–2/2–002 of the Reactor Theory Division, Atomic Energy Corporation of South Africa (1987).

[20] SMITH K S: "An Analytic Nodal Method for Solving the Two–Group Multidimensional Static and Transient Neutron Diffusion Equations". Nucl. Eng. Thesis, Dept. Nucl., Eng., MIT (1979).

[21] PARSONS D K and NIGG D W: "Extension of the Analytic Nodal Method to Four Energy Groups". EGG–PBS–6821 (1985).

[22] DOUGLAS S R: "Energy Condensation and Discontinuity Factors". Report AECL–8771 (1985).

[23] LINDAHL S–O and WEISS Z: "The Response Matrix Method". Advances in Nuclear Science and Technology, Vol. 13. Plenum Press, 1981.

APPENDIX A

THE FEW–GROUP ANALYTIC DIFFUSION THEORY METHOD

This appendix deals with the derivation of the analytic solution to the few–group diffusion equation for a one–dimensional (slab) finite homogeneous medium. General up– and down–scattering between all groups is allowed. This generality is usually not present in other few–group analytic diffusion methods[20,21]. The method presented in this appendix is similar to Bonalumi's[11] method and has been numerically implemented by Weiss[12]. In some respects the method used by Douglas[22] is also similar, except that the present treatment is not limited to diagonal diffusion coefficients.

Consider a homogenised slab node of thickness h. By adopting a local dimensionless coordinate system

$$\xi = \frac{2(u - u_0)}{h} \quad \left[(u^- \le u \le u^+ \;\; ; \;\; u_0 = \tfrac{1}{2}\left[u^- + u^+\right]\right] \quad . \tag{A.1}$$

The equivalent 1–D diffusion equation for the node can be written as

$$\nabla_\xi^2 \langle G|\phi(\xi)\rangle + \sum_{G'} \langle G|B^2|G'\rangle\langle G'|\phi(\xi)\rangle = 0 \quad , \tag{A.2}$$

$$(-1 \le \xi \le +1)$$

$$(G = 1,\ldots,K)$$

$$-\sum_{G'} \langle G|d|G'\rangle\langle G'|\nabla_\xi\phi(\xi)\rangle\Big|_{\xi=\pm1} = \langle G|J(\xi=\pm1)\rangle = \langle G|J^\pm\rangle \quad . \tag{A.3}$$

The real dimensionless diffusion coefficient and buckling matrices are defined by

$$\hat{d} = \frac{2\hat{D}}{h} \quad , \tag{A.4}$$

$$\hat{B}^2 = -\frac{h^2}{4}\,\hat{D}^{-1}\left[\hat{\Sigma}_t^{hom} - \hat{\Sigma}_s^{hom} - \frac{1}{\lambda}\hat{F}^{hom}\right] \tag{A.5}$$

Note that it is not assumed that the diffusion coefficient matrix is diagonal. Non–diagonal diffusion coefficient matrices can, for instance, be calculated from P_1 scattering matrices and total cross sections when these arc available. Non–diagonal $\hat{D}$'s are also readily obtained from certain response matrices[11,12].

The analytic solution to Eq. (A.2) requires the calculation of functions of matrices. In order to make such calculations numerically viable, the diffusion equation for the node is diagonalised by transforming from the K–dimensional group representation to the K–dimensional buckling representation. The buckling representation is defined as the representation in which the eigenkets of the buckling operator $\left[B^2\right]$ are used as basis kets. This requires the solution of the following eigenvalue problem:

$$\sum_{G'} \langle G|B^2|G'\rangle\langle G'|\beta_k\rangle = b_k^2\,\langle G|\beta_k\rangle \qquad (k = 1,\ldots,K) \quad . \tag{A.6}$$

From this solution one obtains the modal matrix $\hat{U}$:

$$\hat{U} = \begin{bmatrix} \langle 1|\beta_1\rangle & \langle 1|\beta_K\rangle \\ \vdots & \vdots \\ \langle K|\beta_1\rangle & \langle K|\beta_K\rangle \end{bmatrix} \quad , \tag{A.7}$$

which, together with its inverse[7],

$$\hat{U}^{-1} = \begin{bmatrix} <\beta_1|1> & <\beta_1|K> \\ \vdots & \cdots \quad \vdots \\ <\beta_K|1> & <\beta_K|K> \end{bmatrix} \quad , \tag{A.8}$$

determines all the transformation coefficients required to convert from the group representation to the buckling representation and vice versa. It is assumed that the eigenkets of the buckling operator span the K–dimensional space in which the K–group diffusion equation is defined.

Now the following similarity transformation can be applied to the diffusion equation in the group representation (Eq. (A.2)):

$$\sum_G <\beta_k|G><G|\phi(\xi)> = <\beta_k|\phi(\xi)> \quad , \tag{A.9}$$

$$\sum_{G,G'} <\beta_{k'}|G><G|B^2|G'><G'|\beta_k> = <\beta_{k'}|B^2|\beta_k> = b_k^2 \quad . \tag{A.10}$$

The result is:

$$\nabla_\xi^2 <\beta_k|\phi(\xi)> + b_k^2 <\beta_k|\phi(\xi)> = 0 \qquad (k = 1,...,K) \quad , \tag{A.11}$$

where the b_k^2's are the eigenvalues of the dimensionless buckling operator B^2. In more than 2 groups these eigenvalues can be complex, but at least one real eigenvalue, b_1^2, exists. The complex eigenvalues and eigenvectors occur in complex conjugate pairs[7].

These K uncoupled Helmholtz equations can each be solved analytically. The exact analytic solution has the following form:

$$<\beta_k|\phi(\xi)> = \frac{\sin b_k(1-\xi)}{\sin 2b_k}<\beta_k|\phi^->\ + \frac{\sin b_k(1+\xi)}{\sin 2b_k}<\beta_k|\phi^+> \qquad (A.12)$$

This expression involves the calculation of functions of constants only.

By transforming Eq. (A.12) back to the group representation, the required few-group analytical solution to Eq. (A.2) is obtained:

$$<G|\phi(\xi)> = \sum_k <G|\beta_k><\beta_k|\phi(\xi)>$$

$$= \sum_{k,G'} <G|\beta_k><\beta_k|\frac{\sin B(1-\xi)}{\sin 2B}|\beta_k><\beta_k|G'><G'|\phi^->$$

$$+ \sum_{k,G'} <G|\beta_k><\beta_k|\frac{\sin B(1+\xi)}{\sin 2B}|\beta_k><\beta_k|G'><G'|\phi^+> \qquad (A.13)$$

$$= \sum_{G'} <G|\frac{\sin B(1-\xi)}{\sin 2B}|G'><G'|\phi^->$$

$$+ \sum_{G'} <G|\frac{\sin B(1+\xi)}{\sin 2B}|G'><G'|\phi^+>$$

In matrix notation:

$$\underset{\sim}{\phi}(\xi) = \frac{\sin \hat{B}(1-\xi)}{\sin 2\hat{B}}\ \underset{\sim}{\phi}^- + \frac{\sin \hat{B}(1+\xi)}{\sin 2\hat{B}}\ \underset{\sim}{\phi}^+ \qquad (A.14)$$

In summary, the procedure for obtaining the few-group analytic diffusion theory solution within a given homogeneous node involves the following steps:

(1) Solve the eigenvalue problem for the dimensionless buckling matrix ($\hat{B}^2$) of the node.

(2) Construct the modal matrix ($\hat{U}$) from the obtained eigenvectors in the group representation and invert it to obtain the inverse modal matrix ($\hat{U}^{-1}$).

(3) For each of the K eigenvalues of the buckling matrix, calculate the analytic flux distribution in the buckling representation (Eq. (A.12)).

(4) Use the modal matrix and its inverse to transform the analytic solution in the buckling representation to the group representation (Eq. (A.13)).

This method of determining the few-group analytic solution to the diffusion equation within a homogenised node is also known[7,12] as the modal expansion method since it involves the expansion of the group fluxes (see Eq. (A,13)) in terms of spatial modes in the buckling representation ($<\beta_k|\phi(\xi)>$), with the expansion coefficients being the elements $<G|\beta_k>$ of the buckling or spectral modes. The buckling mode corresponding to the largest (least negative) real eigenvalue b_1^2 of the buckling matrix B has all positive and real elements and is called the fundamental mode spectrum. Similarly, the spatial mode corresponding to the fundamental mode buckling eigenvalue is referred to as the fundamental mode spatial distribution.

For a multiplying node in which $\lambda < k_\infty$, the fundamental eigenvalue b_1^2 is positive, while it is negative if $\lambda > k_\infty$. It is always negative for non-multiplying nodes. The remaining k-1 eigenvalues all have negative real parts.

The fundamental spatial mode dominates all the other modes in its contribution to the group flux distribution within the node. The remaining spatial modes are called transient modes since they decay rapidly away from the node faces towards the node interior and hence contribute mainly to the spatial transients in the group fluxes near nodal interfaces.

APPENDIX B

DERIVATION OF THE T-RESPONSE MATRIX RELATION

The T-response matrix[23] relates the normal outgoing gradients of the flux on the boundaries of a node to the flux values at these boundaries. The derivation of this relationship based on the few-group analytic diffusion theory flux solution within a homogenised slab node is straightforward. Simple differentiation of the matrix equation, Eq. (A.14), and evaluation of the result at $\xi = \pm 1$ would directly yield the desired relationship. However, for numerical calculation of the elements of the T-response matrix one must first calculate certain functions of the buckling operator in the buckling representation. In other words, the T-response must first be computed in the buckling representation.

In order to derive the T-response in the buckling representation, Eq. (A.12) is differentiated with respect to ξ and evaluated at $\xi = \pm 1$:

$$\begin{aligned} \langle \bar{\beta}_k | \phi_n^- \rangle &= c(b_k) \langle \bar{\beta}_k | \phi^- \rangle - p(b_k) \langle \bar{\beta}_k | \phi^+ \rangle \quad , \\ \langle \bar{\beta}_k | \phi_n^+ \rangle &= -p(b_k) \langle \bar{\beta}_k | \phi^- \rangle + c(b_k) \langle \bar{\beta}_k | \phi^+ \rangle \quad . \end{aligned} \qquad (k = 1,\ldots,K) \qquad (B.1)$$

Here $|\phi_n^{\pm}\rangle$ represents the outward normal derivative of $|\phi(\xi)\rangle$ at $\xi = \pm 1$ and

$$c(b_k) = \frac{b_k}{\tan 2b_k} \quad , \qquad (B.2)$$

$$p(b_k) = \frac{b_k}{\sin 2b_k} \quad . \qquad (B.3)$$

In matrix notation, the T–response relation in the buckling representation is written as

$$\langle \bar{\beta}_k | \underline{\phi}_n \rangle = \underline{\underline{T}}(b_k) \langle \bar{\beta}_k | \underline{\phi} \rangle = \langle \bar{\beta}_k | \underline{\underline{T}}(B) | \underline{\phi} \rangle \quad , \tag{B.4}$$

where

$$|\underline{\phi}_n\rangle = \begin{bmatrix} |\phi_n^-\rangle \\ |\phi_n^+\rangle \end{bmatrix} \quad ,$$

$$|\underline{\phi}\rangle = \begin{bmatrix} |\phi^-\rangle \\ |\phi^+\rangle \end{bmatrix} \quad , \tag{B.5}$$

and

$$\underline{\underline{T}}(b_k) = \begin{bmatrix} c(b_k) & -p(b_k) \\ -p(b_k) & c(b_k) \end{bmatrix} \quad .$$

The T–response relation in the buckling representation can now be transformed to the group representation:

$$\langle G | \underline{\phi}_n \rangle = \sum_k \langle G | \beta_k \rangle \langle \bar{\beta}_k | \underline{\phi}_n \rangle$$

$$= \sum_{k,G'} \langle G | \beta_k \rangle \langle \bar{\beta}_k | \underline{\underline{T}}(B) | \beta_k \rangle \langle \bar{\beta}_k | G' \rangle \langle G' | \underline{\phi} \rangle \tag{B.6}$$

$$= \sum_{G'} \langle G | \underline{\underline{T}}(B) | G' \rangle \langle G' | \underline{\phi} \rangle$$

In matrix notation, the well-known[23] slab T-response matrix equation is:

$$\underline{\underline{\tilde{\phi}}}_n = \underline{\underline{\hat{T}}}\ \underline{\underline{\tilde{\phi}}} \quad , \tag{B.7}$$

where

$$\underline{\underline{\tilde{\phi}}}_n = \begin{bmatrix} \tilde{\phi}^-_n \\ \tilde{\phi}^+_n \end{bmatrix} \quad ,$$

$$\underline{\underline{\tilde{\phi}}} = \begin{bmatrix} \tilde{\phi}^- \\ \tilde{\phi}^+ \end{bmatrix} \quad , \tag{B.8}$$

$$\underline{\underline{\hat{T}}} = \begin{bmatrix} \hat{c} & -\hat{p} \\ -\hat{p} & \hat{c} \end{bmatrix} \quad ,$$

and

$$\hat{c} = \begin{bmatrix} <1|c(B)|1> & \cdots & <1|c(B)|K> \\ \vdots & & \\ <K|c(B)|1> & & <K|c(B)|K> \end{bmatrix} \quad , \tag{B.9}$$

$$<G|c(B)|G'> = \sum_k <G|\beta_k><\beta_k|c(B)|\beta_k><\beta_k|G'> \quad .$$

By direct inversion of the 2Kx2K T-response matrix in the group representation, one obtains the group boundary fluxes in terms of the normal outgoing boundary currents:

$$\underline{\underline{\tilde{\phi}}} = \underline{\underline{\hat{T}}}^{-1}\ \underline{\underline{\tilde{\phi}}}_n = -\underline{\underline{\hat{T}}}^{-1}\ \underline{\underline{\hat{d}}}^{-1}\ \underline{\underline{\tilde{J}}}_n \quad . \tag{B.10}$$

Here

$$\underline{\underline{\hat{d}}}^{-1} = \begin{bmatrix} \hat{d}^{-1} & \hat{0} \\ \hat{0} & \hat{d}^{-1} \end{bmatrix} , \tag{B.11}$$

$$\underline{\tilde{J}}_n = \begin{bmatrix} \tilde{J}_n^- \\ \tilde{J}_n^+ \end{bmatrix} .$$

Another way of inverting the T-response matrix is to invert first in the buckling representation prior to transforming to the group representation. This would involve inverting the K matrices, $\underline{\underline{T}}(b_k)$, of Eq. (B.5), each of which is only a 2x2 matrix.

APPENDIX C

THE DIRECT CALCULATION OF THE T^{-1}–RESPONSE MATRIX

The inverse to the T–response matrix can be calculated directly from the FVW cross section of a homogeneous node without the need to first calculate the T–response matrix. To determine the definition of the elements of the T^{-1}–response matrix in terms of functions of the buckling matrix, we start by transforming the T–response matrix:

$$\underline{\underline{\hat{T}}} = \begin{bmatrix} \hat{c} & -\hat{p} \\ -\hat{p} & \hat{c} \end{bmatrix} = \begin{bmatrix} \hat{c}+\hat{p} & \hat{0} \\ \hat{0} & \hat{c}+\hat{p} \end{bmatrix} - \begin{bmatrix} \hat{p} & \hat{p} \\ \hat{p} & \hat{p} \end{bmatrix} \quad . \tag{C.1}$$

Then

$$\begin{aligned} \tilde{\phi}_n^- &= (\hat{c}+\hat{p})\,\tilde{\phi}^- - \hat{p}\,(\tilde{\phi}^- + \tilde{\phi}^+) \quad , \\ \tilde{\phi}_n^+ &= (\hat{c}+\hat{p})\,\tilde{\phi}^+ - \hat{p}\,(\tilde{\phi}^- + \tilde{\phi}^+) \quad , \end{aligned} \tag{C.2}$$

so that

$$\begin{aligned} \tilde{\phi}^- &= (\hat{c}+\hat{p})^{-1}\left[\tilde{\phi}_n^- + \hat{p}\,(\tilde{\phi}^- + \tilde{\phi}^+)\right] \\ &= (\hat{c}+\hat{p})^{-1}\left[-\hat{d}^{-1}\,\tilde{J}_n^- + \hat{p}\,(\tilde{\phi}^- + \tilde{\phi}^+)\right] \quad , \end{aligned} \tag{C.3}$$

$$\begin{aligned} \tilde{\phi}^+ &= (\hat{c}+\hat{p})^{-1}\left[\tilde{\phi}_n^+ + \hat{p}\,(\tilde{\phi}^- + \tilde{\phi}^+)\right] \\ &= (\hat{c}+\hat{p})^{-1}\left[-\hat{d}^{-1}\,\tilde{J}_n^+ + \hat{p}\,(\tilde{\phi}^- + \tilde{\phi}^+)\right] \quad . \end{aligned}$$

From the integration of Eq. (A.14) over the node width, one finds that,

$$\tilde{\phi}^{av} = \frac{\tan \hat{B}}{\hat{B}} \frac{(\tilde{\phi}^{-} + \tilde{\phi}^{+})}{2} \quad . \tag{C.4}$$

Using this result in Eq. (C.3) yields

$$\begin{aligned} \tilde{\phi}^{-} &= \frac{2\hat{B}}{\sin 2\hat{B}} \tilde{\phi}^{av} - \frac{\tan \hat{B}}{\hat{B}} \hat{d}^{-1} \tilde{J}_n^{-} \quad , \\ \tilde{\phi}^{+} &= \frac{2\hat{B}}{\sin 2\hat{B}} \tilde{\phi}^{av} - \frac{\tan \hat{B}}{\hat{B}} \hat{d}^{-1} \tilde{J}_n^{+} \quad . \end{aligned} \tag{C.5}$$

If one integrates the dimensionless diffusion equation for the node (Eq. (A.2)) over the width of the node, the result is

$$\tilde{\phi}^{av} = \frac{1}{\hat{B}^2} \frac{\left[\tilde{\phi}_n^{-} + \tilde{\phi}_n^{+}\right]}{2} \quad . \tag{C.6}$$

This leads to

$$\begin{aligned} \tilde{\phi}^{-} &= \frac{1}{\hat{B} \tan 2\hat{B}} \hat{d}^{-1} \tilde{J}_n^{-} + \frac{1}{\hat{B} \sin 2\hat{B}} \hat{d}^{-1} \tilde{J}_n^{+} \quad , \\ \tilde{\phi}^{+} &= \frac{1}{\hat{B} \sin 2\hat{B}} \hat{d}^{-1} \tilde{J}_n^{-} + \frac{1}{\hat{B} \tan 2\hat{B}} \hat{d}^{-1} \tilde{J}_n^{+} \quad , \end{aligned} \tag{C.7}$$

or, in matrix notation

$$\underline{\tilde{\phi}} = \hat{\underline{\underline{H}}} \underline{\tilde{\phi}}_n = -\hat{\underline{\underline{H}}} \hat{d}^{-1} \underline{\tilde{J}}_n \quad , \tag{C.8}$$

with

$$\hat{\underline{\underline{H}}} = \begin{bmatrix} \hat{q} & \hat{r} \\ \hat{r} & \hat{q} \end{bmatrix} \quad . \tag{C.9}$$

Comparison with Eq. (B.10) leads to the conclusion that

$$\hat{\underline{\underline{T}}}^{-1} = \hat{\underline{\underline{H}}} \quad , \tag{C.10}$$

$$\hat{\underline{\underline{H}}}^{-1} = \hat{\underline{\underline{T}}} \quad .$$

APPENDIX D

THE R–RESPONSE MATRIX

The R–response matrix[23] relates partial currents at nodal boundaries and not fluxes and flux gradients. It is therefore not limited to diffusion theory. The R–response matrix can be calculated directly from transport theory results or from diffusion theory group constants. The present work is limited to diffusion theory, and as a result only the calculation of the elements of the R–matrix from diffusion theory group constants is considered here.

For a homogeneous slab node, the basic R–response relation is

$$\underset{\sim}{\tilde{J}}_n^{(out)} = \hat{\underline{\underline{R}}}\, \underset{\sim}{\tilde{J}}_n^{(in)} \quad , \tag{D.1}$$

where

$$\underset{\sim}{\tilde{J}}_n^{(in)} = \begin{bmatrix} \tilde{J}_n^{(in)-} \\ \tilde{J}_n^{(in)+} \end{bmatrix} \quad ,$$

$$\hat{\underline{\underline{R}}} = \begin{bmatrix} \hat{a} & \hat{t} \\ \hat{t} & \hat{a} \end{bmatrix} \quad . \tag{D.2}$$

The KxK matrix $\hat{a}$ is called the albedo or reflection matrix and $\hat{t}$ is called the transmission matrix. These matrices are functions of the buckling matrix as well as the diffusion matrix of the node and hence they cannot be calculated in the buckling representation as is the case with the T– and T^{-1}–response matrices. The functional form of the albedo and transmission matrices in terms of the diffusion

theory cross sections of a homogenised slab node of size h may be derived from the relationship between the R and T matrices. Using the diffusion theory expressions for partial currents,

$$\begin{aligned} \tilde{\underline{j}}_n^{(out)} &= \frac{1}{4}\hat{E}\,\tilde{\underline{\phi}} - \frac{1}{2}\hat{d}\,\tilde{\underline{\phi}}_n \quad , \\ \tilde{\underline{j}}_n^{(in)} &= \frac{1}{4}\hat{E}\,\tilde{\underline{\phi}} + \frac{1}{2}\hat{d}\,\tilde{\underline{\phi}}_n \quad , \end{aligned} \tag{D.3}$$

together with the T–response matrix relation (Eq. (B.7)), leads to

$$(\hat{\underline{\underline{E}}} - 2\hat{\underline{\underline{d}}}\,\hat{\underline{\underline{T}}})\,\tilde{\underline{\phi}} = \hat{\underline{\underline{R}}}(\hat{\underline{\underline{E}}} + 2\hat{\underline{\underline{d}}}\,\hat{\underline{\underline{T}}})\,\tilde{\underline{\phi}} \quad . \tag{D.4}$$

Since this is valid for arbitrary interface fluxes,

$$\hat{\underline{\underline{R}}} = (\hat{\underline{\underline{E}}} - 2\hat{\underline{\underline{d}}}\,\hat{\underline{\underline{T}}})(\hat{\underline{\underline{E}}} + 2\hat{\underline{\underline{d}}}\,\hat{\underline{\underline{T}}})^{-1} \quad . \tag{D.5}$$

Inversely,

$$\hat{\underline{\underline{T}}} = \frac{1}{2}\,\hat{\underline{\underline{d}}}^{-1}(\hat{\underline{\underline{E}}} + \hat{\underline{\underline{R}}})^{-1}(\hat{\underline{\underline{E}}} - \hat{\underline{\underline{R}}}) \quad . \tag{D.6}$$

From Eq. (D.5),

$$(\hat{\underline{\underline{E}}} - 2\hat{\underline{\underline{d}}}\,\hat{\underline{\underline{T}}}) = \hat{\underline{\underline{R}}}(\hat{\underline{\underline{E}}} + 2\hat{\underline{\underline{d}}}\,\hat{\underline{\underline{T}}}) \quad . \tag{D.7}$$

Substitute Eq. (D.6) into the left–hand side of Eq. (D.7) to obtain

$$(\hat{\underline{\underline{E}}} + \hat{\underline{\underline{R}}})(\hat{\underline{\underline{E}}} + 2\hat{\underline{\underline{d}}}\,\hat{\underline{\underline{T}}}) = 2\hat{\underline{\underline{E}}} \quad . \tag{D.8}$$

This implies

$$(\hat{E} + \hat{a})\,(\hat{E} + 2\hat{d}\,\hat{c}) - 2\hat{t}\,\hat{d}\,\hat{p} = 2\hat{E} \quad ,$$
$$(\hat{E} + \hat{a})\,(-2\hat{d}\,\hat{p}) + \hat{t}\,(\hat{E} + 2\hat{d}\,\hat{c}) = \hat{0} \quad . \tag{D.9}$$

Subtraction and addition of these two equations result in

$$\hat{a} - \hat{t} = [\hat{E} - 2\hat{d}\,(\hat{c} + \hat{p})]\,[\hat{E} + 2\hat{d}\,(\hat{c} + \hat{p})]^{-1} \quad ,$$
$$\hat{a} + \hat{t} = [\hat{E} - 2\hat{d}\,(\hat{c} - \hat{p})]\,[\hat{E} + 2\hat{d}\,(\hat{c} - \hat{p})]^{-1} \quad . \tag{D.10}$$

Solving for $\hat{a}$ and $\hat{t}$:

$$\hat{a} = \left[\hat{E} + (2\hat{d}\hat{B})^2\right]\left[\hat{E} - (2\hat{d}\hat{B})^2 + 2\hat{d}\frac{2\hat{B}}{\tan\,2\hat{B}}\right]^{-1} \quad , \tag{D.11}$$

$$\hat{a} = \left[2\hat{d}\frac{2\hat{B}}{\tan\,2\hat{B}}\right]\left[\hat{E} - (2\hat{d}\hat{B})^2 + 2\hat{d}\frac{2\hat{B}}{\tan\,2\hat{B}}\right]^{-1} \quad . \tag{D.12}$$

These two expressions can be used to calculate the albedo and transmission matrices in the group representation. However, in practice it is easier to calculate $\hat{a}-\hat{t}$ and $\hat{a}+\hat{t}$ and to determine $\hat{a}$ and $\hat{t}$ from these results.

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