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**SYSTEMATIC ASSEMBLY HOMOGENIZATION AND LOCAL FLUX
RECONSTRUCTION FOR NODAL METHOD CALCULATIONS**

Final Report

January 1, 1990 - September 30, 1992

Submitted to:

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**SEAS Report No. UVA/527406/MANE93/102
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**Nuclear Reactor Facility
DEPARTMENT OF MECHANICAL, AEROSPACE
AND NUCLEAR ENGINEERING**

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ENGINEERING
& APPLIED SCIENCE

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EXECUTIVE SUMMARY

The work done under the Department of Energy Grant No. DE-FG02-90ER12931, "Systematic Assembly Homogenization and Local Flux Reconstruction for Nodal Methods Calculations" was completed on September 30, 1992. The research done under this grant included the development of the first systematic simultaneous lattice-cell and fuel-assembly homogenization theory. This homogenization theory provides both a general theoretical framework and an explicit practical procedure within which global (whole-reactor) diffusion calculations, fuel assembly diffusion calculations, and lattice-cell transport calculations can be systematically combined, following explicitly derived mathematical procedures, so that global *diffusion* calculations carried out using very coarse computational meshes will yield values of k_{eff} that are equal to the *transport* theory values within a fourth order error in a small parameter (the ratio of the total mean free path to the characteristic reactor core dimension -- typically 10^{-3} for a light water thermal reactor), and values of the reconstructed angular flux that are equal to the transport theory fluxes to within a first order error in this small parameter. Specifically, this makes it possible to do reactor calculations, using coarse-mesh nodal diffusion methods with fuel-assembly size computational elements or nodes, that will yield results that are comparable to fine-mesh nodal transport results when the diffusion coefficients, cross sections, and flux discontinuity factors used in the nodal diffusion calculations are constructed according to the simple procedures that follow from the new systematic homogenization theory.

The systematic homogenization theory first was applied to simple one-dimensional problems in which the core was made up of various types of fuel assemblies, and the fuel assemblies were comprised of various types of lattice cells; the results of the coarse-mesh nodal diffusion calculations done using the appropriate homogenized diffusion coefficients and cross sections and flux discontinuity factors were compared to the detailed nodal transport calculations, done using sub-fuel-pin size computational elements, to validate the homogenization theory and nodal method computational procedures. Then these computational procedures were applied to various practical two-dimensional PWR problems, including a core made up of 193 fuel assemblies of five types, each comprised of 256 lattice cells. The results showed that the coarse-mesh nodal diffusion calculations based on the systematic homogenization theory yielded results for k_{eff} and assembly powers in better agreement with the results of the detailed two-dimensional nodal transport calculations than did calculations using traditional homogenization procedures or calculations using recently developed homogenization procedures based on so-called equivalence theory or the various improvements, such as generalized equivalence theory, that followed it.

Finally, since many practical reactor calculations begin from diffusion theory bases, a separate systematic homogenization theory starting from the diffusion equation instead of the transport equation also was developed. This homogenization theory and the computational procedures based on it also were validated by first applying it to simple one-dimensional test problems for which the results of the assembly-size-mesh nodal diffusion calculations carried out in the context of the diffusion-equation-based systematic

homogenization theory were compared with detailed fine mesh nodal diffusion calculations. Assembly-size-mesh nodal diffusion calculations using diffusion coefficients, cross sections, and flux discontinuity factors based on the systematic homogenization theory then were done for practical two-dimensional PWR problems, again including the core made up of 193 fuel assemblies of five types, each comprised of 256 lattice cells. The results of these calculations were compared with those of coarse-mesh nodal diffusion calculations based on traditional homogenization procedures and based on generalized equivalence theory; and those obtained via this diffusion-equation-based systematic homogenization theory were significantly more accurate with respect to the reference solutions generated via fine-mesh nodal diffusion calculations done using a sub-lattice-cell-size mesh.

SYSTEMATIC ASSEMBLY HOMOGENIZATION AND LOCAL FLUX
RECONSTRUCTION FOR NODAL METHOD CALCULATIONS

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ABSTRACT

Starting from the transport equation, a systematic theory has been developed for the simultaneous homogenization of lattice cells and fuel assemblies, using multiple scales asymptotic expansion methods. The three-scales introduced correspond to the lattice-cell scale, the full-assembly scale, and the reactor core scale. The resulting global or whole-reactor *diffusion* equation with homogenized diffusion coefficients and cross sections and homogenized-fuel-assembly flux discontinuity factors yields values for k_{eff} that are equivalent to the exact *transport* theory value to within a fourth order error in a small parameter (ratio of the total mean free path to the characteristic reactor dimension), and reconstructed angular fluxes that are equivalent to the transport theory fluxes to within a first order error in that small parameter.

The systematic homogenization theory, which is based on the transport equation, provides a framework within which the full advantages of coarse-mesh nodal diffusion methods can be realized since these computational methods yield extremely accurate results when applied on very coarse meshes. Hence, it was tested and applied using the coarse-mesh Nodal Green's Function Method to do the global (whole-reactor) diffusion calculations on fuel-assembly-sized meshed, and to do the fuel-assembly diffusion calculations on lattice-cell-sized meshes necessary to homogenize the assemblies. The Discrete Nodal Transport Method was used to do the lattice-cell transport calculations necessary to homogenize the cells, and also to do the global transport calculations on sub-lattice-cell-size fine meshes to generate the reference solutions with which comparisons were made. The results of comparisons for practical large two-dimensional PWR cores showed that the nodal diffusion calculations, done on fuel-assembly-size meshes using the diffusion coefficients, cross sections, and fuel-assembly flux discontinuity factors based on the systematic homogenization theory, yielded values for k_{eff} and assembly powers that were considerably more accurate in comparison with the fine-mesh nodal transport values than those obtained using traditional homogenization procedures or the recently developed generalized equivalence theory.

Finally, because the core analysis of thermal reactors sometimes begins from a diffusion theory model, a second systematic homogenization theory -- one that starts from the diffusion equation -- also was developed. It also was applied to practical two-dimensional PWR cores in a manner analogous to way the transport-equation-based systematic homogenization was applied, but with fine-mesh diffusion theory calculations used to provide the reference solutions. The results for k_{eff} and assembly powers obtained via the

diffusion-equation-based systematic homogenization theory, in concert with nodal diffusion calculations done on fuel-assembly-size meshes, were in considerably better agreement with the fine-mesh nodal diffusion values than those obtained via traditional flux and volume weighted homogenization procedures or generalized equivalence theory.

PREFACE

The report is divided into three parts. The main mathematical development of the new systematic simultaneous lattice-cell and fuel-assembly homogenization theory derived from the transport equation is summarized in Part I. Also included in Part I is the validation of this systematic homogenization theory and the resulting calculational procedures for coarse-mesh nodal diffusion methods that follow from it, in the form of their application to a simple one-dimensional test problem.

The results of the application of this transport-equation-based systematic homogenization theory are summarized in Part II in which its superior accuracy over traditional flux and volume weighted homogenization procedures and over generalized equivalence theory is demonstrated for small and large practical two-dimensional PWR problems.

The mathematical development of a second systematic homogenization theory -- this one derived starting from the diffusion equation -- is summarized in Part III where its application to a practical two-dimensional PWR model also is summarized and its superior accuracy over traditional homogenization methods and generalized equivalence theory is demonstrated for this problem.

Finally, the main results of the research done under this grant are reiterated briefly in a short summary that follows the third part of this final report.

PART I: SYSTEMATIC CELL AND ASSEMBLY HOMOGENIZATION AND LOCAL FLUX
RECONSTRUCTION FOR NODAL DIFFUSION METHODS

ABSTRACT OF PART I

A simultaneous pin lattice cell and fuel bundle homogenization theory has been developed for use with nodal diffusion calculations of practical reactors, i.e., large near-critical heterogeneous systems comprised of two-dimensional near-periodic pin lattices and two-dimensional near-periodic arrays of fuel bundles. The theoretical development of the homogenization theory, which is based on multiple-scales asymptotic expansion methods carried out through fourth order in a small parameter, starts from the transport equation and systematically yields: a cell-homogenized bundle diffusion equation with self-consistent expressions for the cell-homogenized cross sections and diffusion tensor elements; and a bundle-homogenized global reactor diffusion equation with self-consistent expressions for the bundle-homogenized cross sections and diffusion tensor elements. The continuity of the angular flux at cell and bundle interfaces leads to jump conditions or so-called discontinuity factors on the scalar flux and also on the net current, or equivalently on the two partial currents, at the cell and bundle interfaces, in terms of the two adjacent cell or bundle eigenfunctions. The solution of the global diffusion equation using nodal methods, in concert with the expressions for the homogenized nuclear data and the flux and current discontinuity factors obtained here, will result in the numerical calculation of the eigenvalue $1/k_{eff}$, using coarse-mesh nodal diffusion methods, that approximates the exact transport theory value to fourth order in the small parameter. The expressions required for the reconstruction of the angular flux or the 'de-homogenization' theory were obtained as an integral part of the

development; hence, the leading order transport theory angular flux is easily reconstructed throughout the reactor including the regions in the interiors of the fuel bundles and the pin lattice cells. The theoretical development shows that the exact transport theory angular flux obtained to leading order from the whole-reactor nodal diffusion calculations, done using the homogenized nuclear data and discontinuity factors, is the product of three computed quantities: a "cell shape function" (the fundamental unit-cell nodal transport theory eigenfunction); a "bundle shape function" (the fundamental cell-homogenized unit-bundle nodal diffusion theory eigenfunction); and a "global shape function" (the fundamental solution to the bundle-homogenized overall reactor nodal diffusion equation). Three numerical examples that illustrate the application of the theoretical results are included. The first, a simple system comprised of periodic cells, verifies that as the system size, i.e., the number of cells, is increased the homogenized diffusion theory results more closely approximate the exact transport theory results. The second and third, both systems comprised of three different assemblies -- one a control assembly and another a partially depleted assembly -- each made up of different periodic cells, show that the homogenization theory leads to accurate values for k_{eff} even when the discontinuity factors are omitted, and that when they are included the deviation from the transport theory value is reduced further.

INTRODUCTION TO PART I

For some years now various nodal diffusion methods have been extensively developed to perform highly accurate and highly efficient practical neutron diffusion calculations^{1,2}. The exceptional accuracy of

these modern nodal methods is most effectively exploited when relatively large coarse-mesh homogenized regions are used in calculations. Hence, the accuracy of these nodal methods usually depends ultimately upon the accuracy of the homogenized parameters being used^{3,4}. Therefore, it/ is essential to provide accurate homogenized parameters if the benefits of nodal diffusion methods are to be truly realized. It is for this reason that various homogenization "prescriptions" have been proposed^{3,4}.

Koebke³ proposed an "Equivalence Theory" based on introducing heterogeneity factors -- along with the traditionally used flux weighted diffusion coefficients and cross sections -- to add more degrees of freedom to reproduce the results of a heterogeneous calculation in the integral sense (node-integrated reaction rates and leakage rates). This approach later was generalized in a "Generalized Equivalence Theory" by Smith⁴, who introduced discontinuity factors. Although the introduction of these heterogeneity factors and discontinuity factors was extremely clever, they have only intuition as a basis and therefore actually are ad hoc. In fact, theoretically they require that the exact heterogeneous global solution be known in advance, although practical approximations that do not require this usually result in sufficiently accurate solutions.

Multiple-scale asymptotic expansion methods have been used previously to establish a systematic theory for lattice cell homogenization. Larsen^{5,6} developed a homogenization theory for periodic lattice cells using two spatial scales. Later, Chiang and Dorning⁷ extended these ideas to two-dimensional near-periodic lattices. Realizing that a lattice cell is far smaller than the optimum size for a coarse-mesh node, Chiang⁸, starting from the conventional multigroup diffusion equation, developed a fuel-bundle-homogenized reactor diffusion equation with bundle-homogenized

parameters. However, an error appears to have been made in that work which resulted in the fortuitous omission of certain cross terms that should have arisen. In the present development, a self-consistent lattice cell and fuel bundle homogenization theory is developed for use with nodal diffusion methods. Motivated by the fact that most reactor cores consist of a large array of fuel bundles each comprised of a large number of lattice cells, the problem is approached by introducing three-spatial scales: the lattice cell (fast) scale; the fuel bundle (medium) scale; and the overall reactor core (slow) scale -- to describe the spatial variation of the flux on the scales of those structures. Asymptotic expansions of the angular flux and the eigenvalue are introduced in powers of a small parameter ϵ , defined as the square root of the ratio of the mean free path $\bar{\lambda}$ to the characteristic reactor dimension R . Substitution of these expansions into the transport equation, followed by fairly extensive mathematical manipulations to carry out the analysis of perturbation hierarchy equations through the fourth order, results in the derivation of three mutually consistent neutron balance equations -- one defined on each of the three relevant engineering units: the cell, the bundle, and the reactor. The zeroth order equation yields the unit cell transport equation which can be solved using a nodal transport method to obtain the forward and adjoint fundamental cell eigenfunctions and other required cell solutions. The second order equation results in the cell-homogenized bundle diffusion equation with consistent cell-homogenized cross sections and diffusion tensor constructed using the cell solutions. This equation can be solved using a nodal diffusion method to obtain the unit bundle fundamental eigenfunction. Finally, the fourth order equation yields the bundle-homogenized diffusion equation for the whole reactor with consistent bundle-homogenized cross

sections and diffusion tensor developed from the bundle eigenfunctions. This global diffusion equation also can be solved using a nodal diffusion method to determine the global flux distribution. The development yields the transport equation eigenvalue $1/k_{eff}$ to fourth order in the small parameter and the leading order solution for the angular flux as the product of three functions -- the lattice cell transport theory eigenfunction, the bundle diffusion theory eigenfunction, and the global diffusion theory solution. Thus, the development provides a self-consistent procedure for the reconstruction of the angular flux within lattice cells and fuel bundles. Finally, the continuity of the leading order angular flux, the reconstructed flux, across the lattice cell and fuel bundle interfaces leads to jump conditions or discontinuity factors in the scalar fluxes and net currents in the cell-homogenized bundle diffusion theory solutions and in the bundle-homogenized global diffusion theory solutions.

Application of the new multiple-scale homogenization theory, using the discrete nodal transport method⁹ for the cell calculations and the nodal Green's function method¹⁰ for the bundle and reactor calculations, to several test problems led to very accurate values for k_{eff} in comparison with the transport theory values in all cases studied. Moreover, utilization of the discontinuity factors led to even more accurate values in all cases. The error in the bundle powers and the cell powers also were small. In the second and third test problems reported below the bundle power errors were less than 0.004 of the total power and the maximum error in the cell powers was less than 0.0052 in comparison with the transport theory values.

THEORY

We begin from the full three-dimensional one-speed transport equation for a large near critical system composed of near-periodic two-dimensional lattices in a near-periodic two-dimensional array of fuel bundles

$$\begin{aligned} \hat{\Omega} \cdot \nabla_{\underline{x}} \psi(\underline{x}, \hat{\Omega}) + \Sigma_T(\underline{x}) \psi(\underline{x}, \hat{\Omega}) = \int_{4\pi} \Sigma_S(\underline{x}, \hat{\Omega} \cdot \hat{\Omega}') \psi(\underline{x}, \hat{\Omega}') d^2\Omega' \\ + \frac{1}{4\pi} \frac{1}{k_{\text{eff}}} \nu \Sigma_f(\underline{x}) \int_{4\pi} \psi(\underline{x}, \hat{\Omega}') d^2\Omega' \end{aligned} \quad (1)$$

and introduce three spatial scales

$$\xi_i = \frac{x_i}{\lambda}, \quad \eta_i = \epsilon \frac{x_i}{\lambda}, \quad i = 1, 2, \text{ and } \zeta_i = \epsilon^2 \frac{x_i}{\lambda}, \quad i = 1, 2, 3$$

The total mean free path $\bar{\lambda}$ is of the order of a lattice cell characteristic dimension and therefore small compared to the fuel bundle dimension and very small compared to the reactor dimension R . Hence, the parameter $\epsilon = \sqrt{\bar{\lambda}/R}$ is small. Introducing these spatial scales and dimensionless cross sections into Eq. (1) results in

$$\begin{aligned} \sqrt{1-\mu^2} \left(\cos\phi \frac{\partial}{\partial \xi_1} + \sin\phi \frac{\partial}{\partial \xi_2} \right) \psi(\xi_1, \xi_2, \underline{\eta}, \underline{\zeta}, \hat{\Omega}) + \epsilon \hat{\Omega} \cdot \nabla_{\underline{\eta}} \psi \\ + \epsilon^2 \hat{\Omega} \cdot \nabla_{\underline{\zeta}} \psi + \sigma_T(\xi_1, \xi_2; \underline{\eta}, \underline{\zeta}) \psi = \int_{4\pi} \sigma_S(\xi_1, \xi_2, \hat{\Omega} \cdot \hat{\Omega}'; \underline{\eta}, \underline{\zeta}) \psi d^2\Omega' \\ + \frac{1}{4\pi} \frac{1}{k_{\text{eff}}} \nu \sigma_f(\xi_1, \xi_2; \underline{\eta}, \underline{\zeta}) \int_{4\pi} \psi d^2\Omega' \end{aligned} \quad (2)$$

where the dimensionless cross sections

$$\sigma_i(\xi_1, \xi_2; \underline{\eta}, \underline{\zeta}) = \bar{\lambda} \Sigma_i(\underline{x}) ; i = s, T, f$$

and other functions that appear below depend only parametrically upon the arguments that follow the semicolons. The near-periodic spatial dependence of the cross sections leads to

$$\sigma_1(\xi_1 + \bar{m}_1, \xi_2; n, \zeta) = \sigma_1(\xi_1, \xi_2; n, \zeta)$$

$$\sigma_1(\xi_1, \xi_2 + \bar{m}_2; n, \zeta) = \sigma_1(\xi_1, \xi_2; n, \zeta)$$

where the dimensionless cell pitch $\bar{m}$ ($= m/\bar{\lambda}$) is order unity.

Expanding ψ and $\frac{1}{k_{\text{eff}}}$ in powers of ϵ

$$\psi(\xi_1, \xi_2, n, \zeta, \hat{\Omega}) = \sum_{n=0}^{\infty} \epsilon^n \psi_n(\xi_1, \xi_2, n, \zeta, \hat{\Omega})$$

$$\frac{1}{k_{\text{eff}}} = \sum_{n=0}^{\infty} \epsilon^n \frac{1}{k_n},$$

substituting in Eq. (2) and setting the coefficients of the various powers of ϵ equal to zero leads to a set of hierarchy equations.

The ϵ^0 order equation is

$$\begin{aligned} F\psi_0(\xi_1, \xi_2, n, \zeta, \hat{\Omega}) &= \sqrt{1-\mu^2} \left(\cos\phi \frac{\partial}{\partial \xi_1} + \sin\phi \frac{\partial}{\partial \xi_2} \right) \psi_0 + \sigma_T(\xi_1, \xi_2; n, \zeta) \psi_0 \\ &- \int_{4\pi} \int_{\Omega'} q_1(\xi_2, \xi_1, \hat{\Omega} \cdot \hat{\Omega}'; n, \zeta) \psi_0 d^2\Omega' \\ &- \frac{1}{k} \nu \sigma(\xi_1, \xi_2; n, \zeta) \int_{4\pi} \psi_0 d^2\Omega' = 0 \end{aligned} \quad (3)$$

The general solution for ψ_0 is

$$\psi_0(\xi_1, \xi_2, n, \zeta, \hat{\Omega}) = A_0(n, \zeta) \psi_0^{(0)}(\xi_1, \xi_2, \hat{\Omega}; n, \zeta) \quad (4)$$

where $\psi_0^{(0)}$ is the "cell eigenfunction" or the fundamental eigenfunction of the unit cell transport equation with periodic boundary conditions [Eq. (3)] corresponding to the fundamental cell eigenvalue $1/k_{0,0}^{n,\zeta}$, both of which depend parametrically upon n and ζ ; and $A_0(n, \zeta)$ is yet to be determined. The equation adjoint to Eq. (3), whose solution $\psi_0^{(0)\dagger}$ will be needed to establish the solvability conditions for the higher order equations, can be written immediately, and it easily follows that

$$\psi_0^{(o)\dagger}(\xi_1, \xi_2, \mu, \phi; \underline{n}, \underline{\zeta}) = \psi_0^{(o)}(\xi_1, \xi_2, \mu, \phi - \pi; \underline{n}, \underline{\zeta}). \quad (5)$$

The ϵ^1 order equation is

$$F \psi_1(\xi_1, \xi_2, \underline{n}, \underline{\zeta}, \hat{\Omega}) = -\hat{\Omega} \cdot \nabla_{\underline{n}} \psi_0 + \frac{1}{4\pi} \frac{1}{k_1} \int_{4\pi} \nu \sigma_f \psi_0 d^2\Omega' \quad (6)$$

By the Fredholm alternative theorem Eq. (6) has a solution if and only if the right hand side is orthogonal to $\psi_0^{(o)\dagger}$. This condition yields

$$-\langle \psi_0^{(o)\dagger}, \hat{\Omega} \cdot \nabla_{\underline{n}} (A_0(\underline{n}, \underline{\zeta}) \psi_0^{(o)}) \rangle_c + \frac{1}{k_1} \langle \psi_0^{(o)\dagger}, \nu \sigma_f A_0 \bar{\psi}_0^{(o)} \rangle_c = 0 \quad (7)$$

where the inner product $\langle \rangle_c$ is the integral over the lattice cell and all $\hat{\Omega}$. In terms of a second entry $\bar{a}$, it is

$$\langle \psi_0^{(o)\dagger}, \bar{a} \rangle_c = \int_{\text{cell}} d^2\xi \int_{4\pi} d^2\Omega \psi_0^{(o)\dagger}(\xi_1, \xi_2, \hat{\Omega}; \underline{n}, \underline{\zeta}) \bar{a}(\xi_1, \xi_2, \underline{n}, \underline{\zeta})$$

where

$$\bar{a} = \frac{1}{4\pi} \int_{4\pi} a(\xi_1, \xi_2, \hat{\Omega}, \underline{n}, \underline{\zeta}) d^2\Omega.$$

Eq. (7) yields

$$\frac{1}{k_1^{\underline{n}, \underline{\zeta}}} = \langle \psi_0^{(o)\dagger}, \hat{\Omega} \cdot \nabla_{\underline{n}} \psi_0^{(o)} \rangle_c / \langle \psi_0^{(o)\dagger}, \nu \sigma_f \bar{\psi}_0^{(o)} \rangle_c \quad (8)$$

where the parametric dependence of k_1 upon $\underline{n}$ and $\underline{\zeta}$ has been indicated. The general solution for ψ_1 is then obtained from Eq. (6) as

$$\begin{aligned} \psi_1(\xi_1, \xi_2, \underline{n}, \underline{\zeta}, \hat{\Omega}) = & A_1(\underline{n}, \underline{\zeta}) \psi_0^{(o)}(\xi_1, \xi_2, \hat{\Omega}; \underline{n}, \underline{\zeta}) \\ & - f(\xi_1, \xi_2, \hat{\Omega}; \underline{n}, \underline{\zeta}) \frac{\partial A_0}{\partial \eta_1} - g(\xi_1, \xi_2, \hat{\Omega}; \underline{n}, \underline{\zeta}) \frac{\partial A_0}{\partial \eta_2} \end{aligned} \quad (9)$$

$$- [f'(\xi_1, \xi_2, \hat{\Omega}; \underline{n}, \underline{\zeta}) + g'(\xi_1, \xi_2, \hat{\Omega}; \underline{n}, \underline{\zeta}) - q(\xi_1, \xi_2, \hat{\Omega}; \underline{n}, \underline{\zeta})] A_0$$

where f, g, f', g' and q satisfy inhomogeneous cell transport equations,

$F_z(\xi_1, \xi_2, \hat{\Omega}; \underline{n}, \zeta) = Q$, with Q given respectively for $z = f, g, f', g'$ and q as

$$\begin{aligned} & \sqrt{1-\mu^2} \cos\phi \psi_o^{(o)}; \quad \sqrt{1-\mu^2} \sin\phi \psi_o^{(o)}; \quad \sqrt{1-\mu^2} \cos\phi \frac{\partial \psi_o^{(o)}}{\partial \eta_1}; \\ & \sqrt{1-\mu^2} \sin\phi \frac{\partial \psi_o^{(o)}}{\partial \eta_2}; \quad \frac{1}{k_1 \underline{n}, \zeta} \nu \sigma_f \bar{\psi}_o^{(o)}. \end{aligned}$$

The ϵ^2 order equation is

$$\begin{aligned} F\psi_2(\xi_1, \xi_2, \underline{n}, \zeta, \hat{\Omega}) = & -\hat{\Omega} \cdot \nabla_{\underline{n}} \psi_1 - \hat{\Omega} \cdot \nabla_{\zeta} \psi_o \\ & + \frac{1}{4\pi} \frac{1}{k_1 \underline{n}, \zeta} \nu \sigma_f \int_{4\pi} \psi_1 d^2\Omega' + \frac{1}{4\pi} \frac{1}{k_2} \nu \sigma_f \int_{4\pi} \psi_o d^2\Omega' \end{aligned} \quad (10)$$

For it to have a solution its right hand side, by the Fredholm alternative theorem, also must be orthogonal to $\psi_o^{(o)\dagger}$. This yields

$$\begin{aligned} & -\langle \psi_o^{(o)\dagger}, \hat{\Omega} \cdot \nabla_{\underline{n}} \psi_1 \rangle_c - \langle \psi_o^{(o)\dagger}, \hat{\Omega} \cdot \nabla_{\zeta} \psi_o \rangle_c \\ & - \langle \psi_o^{(o)\dagger}, \frac{1}{k_1 \underline{n}, \zeta} \nu \sigma_f \bar{\psi}_1 \rangle_c + \langle \psi_o^{(o)\dagger}, \frac{1}{k_2} \nu \sigma_f \bar{\psi}_o \rangle_c = 0 \end{aligned} \quad (11)$$

Rearranging this equation, we obtain the cell-homogenized diffusion equation for the fuel bundle

$$\begin{aligned} LA_o(\underline{n}, \zeta) = & \nabla_{\underline{n}} \cdot \underline{D}_c \cdot \nabla_{\underline{n}} A_o(\underline{n}, \zeta) + \frac{1}{k_2} \overline{\nu \sigma_f} A_o \\ & + \underline{T}_c \cdot \nabla_{\underline{n}} A_o + \Lambda_c A_o = 0 \end{aligned} \quad (12)$$

where the cell-homogenized diffusion tensor and cross section in Eq.(12) are

$$\underline{D}_c = \begin{bmatrix} \langle \psi_o^{(o)\dagger}, \sqrt{1-\mu^2} \cos\phi f \rangle_c & \langle \psi_o^{(o)\dagger}, \sqrt{1-\mu^2} \cos\phi g \rangle_c \\ \langle \psi_o^{(o)\dagger}, \sqrt{1-\mu^2} \sin\phi f \rangle_c & \langle \psi_o^{(o)\dagger}, \sqrt{1-\mu^2} \sin\phi g \rangle_c \end{bmatrix}$$

and

$$\overline{\nu\sigma}_f = \langle \psi_o^{(o)\dagger}, \nu\sigma_f \bar{\psi}_o^{(o)} \rangle_c.$$

The last two terms in Eq. (12) are the previously known^{6,7} drift term and source (or sink) term, and their coefficients are omitted here.

The general solution of Eq. (12) for A_o is

$$A_o(\eta, \zeta) = a_o(\zeta) \theta_o^{(o)}(\eta; \zeta) \quad (13)$$

where $\theta_o^{(o)}(\eta; \zeta)$ is the "bundle eigenfunction" or the fundamental eigenfunction of Eq. (12) corresponding to the fundamental eigenvalue $\frac{1}{k_{2,0}^{\zeta}}$; and $a_o(\zeta)$ is yet to be determined. The general solution for ψ_2 is

$$\begin{aligned} \psi_2(\xi_1, \xi_2, \eta, \zeta, \hat{\Omega}) &= A_2(\eta, \zeta) \psi_o^{(o)}(\xi_1, \xi_2, \hat{\Omega}; \eta, \zeta) - f \frac{\partial A_1}{\partial \eta_1} - g \frac{\partial A_1}{\partial \eta_2} \\ &- (f' + g' - q)A_1 + f_1 \frac{\partial^2 A_o}{\partial \eta_1^2} + g_1 \frac{\partial^2 A_o}{\partial \eta_1 \partial \eta_2} + f_2 \frac{\partial^2 A_o}{\partial \eta_2^2} + P_1 \frac{\partial A_o}{\partial \eta_1} \\ &+ P_2 \frac{\partial A_o}{\partial \eta_2} + ZA_o - f \frac{\partial A_o}{\partial \zeta_1} - g \frac{\partial A_o}{\partial \zeta_2} - h \frac{\partial A_o}{\partial \zeta_3} \end{aligned}$$

where $f_1, g_1, f_2, P_1, P_2, h$ and Z satisfy the inhomogeneous cell transport equations $Fz(\xi_1, \xi_2, \hat{\Omega}; \eta, \zeta) = Q$, with Q given respectively for z

$= f_1, \dots, Z$ as

$$\sqrt{1-\mu^2} \cos\phi f; \quad \sqrt{1-\mu^2} (\sin\phi f + \cos\phi g); \quad \sqrt{1-\mu^2} \sin\phi g;$$

$$\hat{\Omega} \cdot \nabla_{\underline{n}} f + \sqrt{1-\mu^2} \cos\phi(f' + g' - q) = \frac{1}{k_1^{\underline{n}, \zeta}} \nu_{\sigma f} \bar{f} ;$$

$$\hat{\Omega} \cdot \nabla_{\underline{n}} g + \sqrt{1-\mu^2} \sin\phi(f' + g' - q) = \frac{1}{k_1^{\underline{n}, \zeta}} \nu_{\sigma f} \bar{g} ; \quad \mu \psi_o^{(o)} ;$$

$$\begin{aligned} \hat{\Omega} \cdot \nabla_{\underline{n}} (f' + g' - q) - \hat{\Omega} \cdot \nabla_{\underline{\zeta}} \psi_o^{(o)} &= \frac{1}{k_{2,0}^{\underline{\zeta}}} \nu_{\sigma f} \bar{\psi}_o^{(o)} \\ &- \frac{1}{k_1^{\underline{n}, \zeta}} \nu_{\sigma f} (\bar{f}' + \bar{g}' - \bar{q}) \end{aligned}$$

Application of the Fredholm alternative for the operator F on the ϵ^3 equation

$$\begin{aligned} F \psi_3(\xi_1, \xi_2, \hat{\Omega}; \underline{n}, \underline{\zeta}) &= -\hat{\Omega} \cdot \nabla_{\underline{n}} \psi_2 - \hat{\Omega} \cdot \nabla_{\underline{\zeta}} \psi_1 \\ &+ \frac{1}{4\pi} \frac{1}{k_1^{\underline{n}, \zeta}} \nu_{\sigma f} \int_{4\pi} \psi_2 d^2\Omega' + \frac{1}{4\pi} \frac{1}{k_2} \nu_{\sigma f} \int_{4\pi} \psi_1 d^2\Omega' \\ &+ \frac{1}{4\pi} \frac{1}{k_3^{\underline{n}, \zeta}} \nu_{\sigma f} \int_{4\pi} \psi_o d^2\Omega' \end{aligned} \quad (14)$$

yields

$$\begin{aligned} -\langle \psi_o^{(o)\dagger}, \hat{\Omega} \cdot \nabla_{\underline{n}} \psi_2 \rangle_c &= \langle \psi_o^{(o)\dagger}, \hat{\Omega} \cdot \nabla_{\underline{\zeta}} \psi_1 \rangle_c + \langle \psi_o^{(o)\dagger}, \frac{1}{k_1^{\underline{n}, \zeta}} \nu_{\sigma f} \psi_2 \rangle_c \\ &+ \langle \psi_o^{(o)\dagger}, \frac{1}{k_{2,0}^{\underline{\zeta}}} \nu_{\sigma f} \bar{\psi}_1 \rangle_c + \langle \psi_o^{(o)\dagger}, \frac{1}{k_3} \nu_{\sigma f} \bar{\psi}_o \rangle_c = 0. \end{aligned} \quad (15)$$

Rewriting this equation, we obtain

$$LA_1 = \gamma(\underline{n}, \underline{\zeta}) a_o(\underline{\zeta}) - \underline{\omega}(\underline{n}, \underline{\zeta}) \cdot \nabla_{\underline{\zeta}} a_o \quad (16)$$

where the operator L is defined in Eq. (12), and because of their length

$\gamma(\underline{n}, \underline{\zeta})$ and $\underline{\omega}(\underline{n}, \underline{\zeta})$ are given in Appendix I-A.

Now, for Eq. (16) to have a solution, its right hand side must be

orthogonal to the eigenfunction of the operator adjoint to L, as a result of the Fredholm alternative theorem. Hence, applying this theorem now for the operator L, not the operator F, yields

$$Ra_o = \langle \theta_o^{(o)\dagger}, \gamma(\underline{n}, \underline{\zeta}) \rangle_b a_o(\underline{\zeta}) - \langle \theta_o^{(o)\dagger}, \underline{\omega}(\underline{n}, \underline{\zeta}) \rangle_b \cdot \nabla_{\underline{\zeta}} a_o = 0 \quad (17)$$

where the inner-product $\langle \rangle_b$ is the integral over the fuel bundle

$$\langle \theta_o^{(o)\dagger}, a(\underline{n}, \underline{\zeta}) \rangle_b = \int_{\text{bundle}} d^2\eta \theta_o^{(o)\dagger}(\underline{n}; \underline{\zeta}) a(\underline{n}, \underline{\zeta}),$$

and $\theta_o^{(o)\dagger}$ is the solution to equation adjoint to Eq. (12). Rearranging Eq. (17) as

$$-\nabla_{\underline{\zeta}} \cdot (\langle \theta_o^{(o)\dagger}, \underline{\omega}(\underline{n}, \underline{\zeta}) \rangle_b a_o) + (\langle \theta_o^{(o)\dagger}, \gamma \rangle_b + \nabla_{\underline{\zeta}} \cdot \langle \theta_o^{(o)\dagger}, \underline{\omega} \rangle_b) a_o = 0, \quad (18)$$

using the boundary condition $a_o(\underline{\zeta}_s) = 0$, and integrating it over the reactor yields

$$\int d^3\zeta [\langle \theta_o^{(o)\dagger}, \gamma(\underline{n}, \underline{\zeta}) \rangle_b + \nabla_{\underline{\zeta}} \cdot \langle \theta_o^{(o)\dagger}, \underline{\omega}(\underline{n}, \underline{\zeta}) \rangle_b] a_o(\underline{\zeta}) = 0. \quad (19)$$

To satisfy Eq. (19), we require that

$$\langle \theta_o^{(o)\dagger}, \gamma(\underline{n}, \underline{\zeta}) \rangle_b + \nabla_{\underline{\zeta}} \cdot \langle \theta_o^{(o)\dagger}, \underline{\omega}(\underline{n}, \underline{\zeta}) \rangle_b = 0 \quad (20)$$

which can be solved to obtain $\frac{1}{k_3^{\underline{\zeta}}}$. The general solution for A_1 is

$$A_1(\underline{n}, \underline{\zeta}) = a_1(\underline{\zeta}) \theta_o^{(o)}(\underline{n}; \underline{\zeta}) + a_o(\underline{\zeta}) v(\underline{n}, \underline{\zeta}) - \underline{r}(\underline{n}, \underline{\zeta}) \cdot \nabla_{\underline{\zeta}} a_o(\underline{\zeta}) \quad (21)$$

where v and $\underline{r}$ satisfy the inhomogeneous cell-homogenized bundle diffusion equations

$$Lv(\underline{n}, \underline{\zeta}) = \gamma(\underline{n}, \underline{\zeta}); \quad L\underline{r}(\underline{n}, \underline{\zeta}) = \underline{\omega}(\underline{n}, \underline{\zeta}).$$

The general solution for ψ_3 is

$$\psi_3(\xi_1, \xi_2, \underline{n}, \underline{\zeta}, \hat{\Omega}) = A_3(\underline{n}, \underline{\zeta}) \psi_o^{(o)}(\xi_1, \xi_2, \hat{\Omega}; \underline{n}, \underline{\zeta}) - f \frac{\partial A_2}{\partial \eta_1} - g \frac{\partial A_2}{\partial \eta_2}$$

$$\begin{aligned}
& -(f' + g' - q)A_2 + f_1 \frac{\partial^2 A_1}{\partial \eta_1^2} + g_1 \frac{\partial^2 A_1}{\partial \eta_1 \partial \eta_2} + f_2 \frac{\partial^2 A_1}{\partial \eta_2^2} + P_1 \frac{\partial A_1}{\partial \eta_1} \\
& + P_2 \frac{\partial A_1}{\partial \eta_2} + ZA_1 - f \frac{\partial A_1}{\partial \zeta_1} - g \frac{\partial A_1}{\partial \zeta_2} - h \frac{\partial A_1}{\partial \zeta_3} + H(\xi_1, \xi_2, \eta, \zeta, \hat{\Omega}, A_0)
\end{aligned}$$

where H is given in Appendix I-B.

The ϵ^4 order equation is

$$\begin{aligned}
F\psi_4(\xi_1, \xi_2, \eta, \zeta, \hat{\Omega}) &= -\hat{\Omega} \cdot \nabla_{\eta} \psi_3 - \hat{\Omega} \cdot \nabla_{\zeta} \psi_2 \\
&+ \frac{1}{4\pi} \frac{1}{k_1} \frac{1}{\eta, \zeta} \nu_{\sigma f} \int_{4\pi} \psi_3^2 d\Omega' + \frac{1}{4\pi} \frac{1}{k_{2,0}} \nu_{\sigma f} \int_{4\pi} \psi_2^2 d\Omega' \\
&+ \frac{1}{4\pi} \frac{1}{k_{3,0}} \nu_{\sigma f} \int_{4\pi} \psi_1^2 d\Omega' + \frac{1}{4\pi} \frac{1}{k_4} \nu_{\sigma f} \int_{4\pi} \psi_0^2 d\Omega'
\end{aligned} \tag{22}$$

Applying the Fredholm alternative for the operator F to Eq. (22) yields

$$\begin{aligned}
-<\psi_o^{(o)\dagger}, \hat{\Omega} \cdot \nabla_{\eta} \psi_3>_c &= <\psi_o^{(o)\dagger}, \hat{\Omega} \cdot \nabla_{\zeta} \psi_2>_c + \frac{1}{k_1} <\psi_o^{(o)\dagger}, \nu_{\sigma f} \bar{\psi}_3>_c \\
&+ <\psi_o^{(o)\dagger}, \nu_{\sigma f} \left(\frac{1}{k_{2,0}} \bar{\psi}_2 + \frac{1}{k_3} \bar{\psi}_1 + \frac{1}{k_4} \bar{\psi}_0 \right)>_c = 0
\end{aligned} \tag{23}$$

Substituting ψ_i , $i = 0, 1, 2, 3$ in Eq. (23) and after substantial manipulations, we obtain an inhomogeneous equation for A_2 ,

$$LA_2 = S(A_0, A_1) \tag{24}$$

where the very long expression for $S(A_0, A_1)$ is given in Appendix I-C.

Applying the Fredholm alternative for operator L to Eq. (24) yields

$$<\psi_o^{(o)\dagger}, S>_b = 0 \tag{25}$$

Substituting A_0 , A_1 and H into Eq. (28), yields the long equation given in Appendix D. Since a_1 appears in this equation, along with a_0 , an additional condition that relates a_1 and a_0 , which can be used to

eliminate a_1 , is necessary. We impose an orthogonality condition^{11,12}

$$\langle \theta_o^{(o)\dagger}, A_1(\underline{r}, \underline{\zeta}) \rangle_b = 0 \quad (26)$$

to obtain

$$a_1(\underline{\zeta}) = [\langle \theta_o^{(o)\dagger}, \theta_o^{(o)} \rangle_b]^{-1} (\langle \theta_o^{(o)\dagger}, \underline{r} \rangle \cdot \nabla_{\underline{\zeta}} a_o - \langle \theta_o^{(o)\dagger}, \underline{v} \rangle a_o).$$

Therefore, the left hand side of Eq. (D-1) in Appendix I-D becomes an equation for a_o . Truncating the expansion of $\frac{1}{k_{eff}}$ at ϵ^4 order

$$\frac{1}{k_4} = \left(\frac{1}{k_{eff}} - \frac{1}{k_{0,0}^{\underline{n}, \underline{\zeta}}} \right) \frac{1}{\epsilon^4} - \left(\frac{1}{k_1^{\underline{n}, \underline{\zeta}}} \epsilon + \frac{1}{k_{2,0}^{\underline{\zeta}}} \epsilon^2 + \frac{1}{k_3^{\underline{\zeta}}} \epsilon^3 \right) \frac{1}{\epsilon^4}$$

and substituting into that equation, we obtain the bundle-homogenized global diffusion equation for the reactor

$$\nabla_{\underline{\zeta}} \cdot \underline{D}_b \cdot \nabla_{\underline{\zeta}} a_o + \frac{1}{\epsilon^4} \left(\frac{1}{k_{eff}} \overline{\nu \sigma_f} - \overline{\sigma_a} \right) a_o + \underline{\Gamma}_b \cdot \nabla_{\underline{\zeta}} a_o + S_b a_o = 0. \quad (27)$$

Here the bundle-homogenized diffusion tensor is

$$\underline{D}_b = \underline{D}_b^o - \underline{D}_b^1 - \underline{D}_b^2 + \underline{D}_b^3$$

where

$$\underline{D}_b^o = \begin{bmatrix} \langle \theta_o^{(o)\dagger}, D_{c_{11}} \theta_o^{(o)} \rangle_b & \langle \theta_o^{(o)\dagger}, D_{c_{12}} \theta_o^{(o)} \rangle_b & 0 \\ \langle \theta_o^{(o)\dagger}, D_{c_{21}} \theta_o^{(o)} \rangle_b & \langle \theta_o^{(o)\dagger}, D_{c_{22}} \theta_o^{(o)} \rangle_b & 0 \\ 0 & 0 & \langle \theta_o^{(o)\dagger}, \langle \psi_o^{(o)\dagger}, \mu \rangle_h \theta_o^{(o)} \rangle_b \end{bmatrix}$$

and the nonzero parts of $\underline{D}_b^1$ and $\underline{D}_b^2$ are

$$\underline{D}_b^1 = \begin{bmatrix} J[fr_1] & J[fr_2] \\ J[gr_1] & J[gr_2] \end{bmatrix}$$

where $J[\ell_i r_i] = \langle \theta_o^{(o)\dagger}, \langle \psi_o^{(o)\dagger}, \hat{n} \cdot \nabla_{\underline{n}}(\ell_i r_i) - \frac{1}{k_1 \underline{n}, \underline{\zeta}} \nu \bar{\sigma}_{f i r_i} \rangle_c \rangle_b$;
 $i = 1, 2$

$$\underline{D}_b^2 = \begin{bmatrix} M[\sqrt{1-\mu^2} \cos \phi, r_1] & M[\sqrt{1-\mu^2} \cos \phi, r_2] \\ M[\sqrt{1-\mu^2} \sin \phi, r_1] & M[\sqrt{1-\mu^2} \sin \phi, r_2] \end{bmatrix}$$

where

$$M[\Omega_i, r_i] = \langle \theta_o^{(o)\dagger}, \langle \psi_o^{(o)\dagger}, \Omega_i (f \frac{\partial r_i}{\partial \eta_1} + g \frac{\partial r_i}{\partial \eta_2} + (f' + g' - q) r_i) \rangle_c \rangle_b$$

$$i = 1, 2$$

and the nonzero elements in $\underline{D}_b^3$ are

$$\underline{D}_b^3 = [\langle \theta_o^{(o)\dagger}, \underline{\omega} \rangle_b \langle \theta_o^\dagger, \underline{x} \rangle_b (\langle \theta_o^{(o)\dagger}, \theta_o \rangle_b)^{-1}].$$

The bundle homogenized cross sections are

$$\overline{\nu \sigma}_f = \langle \theta_o^{(o)\dagger}, \overline{\nu \sigma}_f \theta_o^{(o)} \rangle_b$$

and

$$\overline{\sigma}_a = \langle \theta_o^{(o)\dagger}, \frac{1}{k_{o,o} \underline{n}, \underline{\zeta}} \overline{\nu \sigma}_f \theta_o^{(o)} \rangle_b.$$

The long expressions for the drift vector and the source (or sink) term are omitted here.

Converting Eq. (27) back to dimensional form, we obtain

$$\nabla_{\underline{x}} \cdot \underline{D}_b \nabla_{\underline{x}} a_o(\underline{x}) + \left(\frac{1}{k_{eff}} - \frac{\overline{\nu \Sigma_f}}{\overline{\Sigma_a}} \right) a_o(\underline{x}) + \underline{\Gamma}_b \cdot \nabla_{\underline{x}} a_o(\underline{x}) + S_b a_o(\underline{x}) = 0 \quad (28)$$

where

$$\underline{D}_b(\underline{x}) = \lambda \underline{D}_b(\underline{\zeta}); \quad \underline{\Gamma}_b(\underline{\omega}) = \epsilon^2 \underline{\Gamma}(\underline{\zeta}); \text{ and } S_b(\underline{x}) = \epsilon^4 S_b(\underline{\zeta})/\bar{\lambda}.$$

Equation (28) is the bundle-homogenized global diffusion equation, to be solved over the whole reactor, that yields the fourth order accurate approximation to the transport equation eigenvalue $1/k_{eff}$. It also gives the leading order solution, in small parameter ϵ , for angular flux over the reactor as $\psi_o = a_o \theta_o^{(o)} \psi_o^{(o)}$. In the next section we discuss the interface conditions at the cell boundaries necessary to solve the cell-homogenized diffusion equation [Eq. (12)] over the fuel bundle and those at the bundle boundaries needed to solve the bundle-homogenized global diffusion equation [Eq. (28)] over the reactor.

INTERFACE CONDITIONS OR DISCONTINUITY FACTORS

It was realized by Koebke³ that the solution of the diffusion equation in a nodal calculation with homogenized parameters and continuity of flux and current conditions at node interfaces, in general, cannot reproduce the node integral reaction rates and the surface averaged leakage rates of a known reference heterogeneous system solution. Thus, he suggested that a jump in the flux at an interface between homogenized nodes be permitted in order for the currents at these interfaces to be equal to those in the heterogeneous system. Hence, so-called equivalence factors -- defined as the ratio of the heterogeneous system flux at the interface to the homogenized system flux at the interface -- were introduced, and a jump interface condition on the flux was proposed.³ The model later was extended by Smith⁴ to permit the

discontinuity of surface averaged fluxes across each nodal interface by defining so-called discontinuity factors.

In the present analysis jump conditions on cell interfaces for the cell-homogenized bundle diffusion equation, and on bundle interfaces for the bundle-homogenized global diffusion equation arise naturally from the theoretical development by requiring continuity of the reconstructed angular flux at all orders at the interfaces. Integration of the resulting zeroth order continuity condition at a bundle interface over all $\hat{\Omega}$ yields the bundle interface flux discontinuity factors for the global diffusion calculation

$$a_o^+ / a_o^- = \theta_o^{(o)-} \bar{\psi}_o^{(o)-} / \theta_o^{(o)+} \bar{\psi}_o^{(o)+} . \quad (29)$$

which have as a special case those previously used⁴. The cell interface flux discontinuity factors are obtained analogously as

$$\theta_o^{(o)+} / \theta_o^{(o)-} = \bar{\psi}_o^{(o)-} / \bar{\psi}_o^{(o)+} . \quad (30)$$

The bundle interface net current discontinuity factors for the global diffusion calculation follow from the continuity of the diffusion theory net current based on the zeroth order reconstructed flux. Integrating this flux over all $\hat{\Omega}$, taking the spatial gradient, forming the scalar product with the diffusion tensor, and taking the limits to a bundle interface yields

$$\begin{aligned} D^{\pm} \cdot \left(\theta_o^{(o)\pm} \bar{\psi}_o^{(o)\pm} \frac{1}{R} \vec{\nabla}_{\xi} a_o^{\pm} + \bar{\psi}_o^{(o)\pm} a_o^{\pm} \left[\frac{1}{\sqrt{\lambda R}} \vec{\nabla}_{\eta} \theta_o^{(o)\pm} \right. \right. \\ \left. \left. + \frac{1}{R} \vec{\nabla}_{\xi} \theta_o^{(o)\pm} \right] + a_o^{\pm} \theta_o^{(o)\pm} \left[\frac{1}{\lambda} \vec{\nabla}_{\xi} \bar{\psi}_o^{(o)\pm} + \frac{1}{\sqrt{\lambda R}} \vec{\nabla}_{\eta} \bar{\psi}_o^{(o)\pm} \right. \right. \\ \left. \left. + \frac{1}{R} \vec{\nabla}_{\xi} \bar{\psi}_o^{(o)\pm} \right] \right) . \end{aligned} \quad (31)$$

Equating the two ($\pm$) limiting values of this expression at the interface gives

the discontinuity factor for the interface net currents $-\underline{D}^{\pm} \cdot \vec{\nabla}_{\underline{r}} a_0^{\pm}$ that arise in the bundle-homogenized global diffusion calculation. The expression that leads to the cell interface discontinuity factors is developed analogously and corresponds to Eq. (31) with $a_0^{\pm}$ set equal to unity. Finally, the discontinuity factors for interface partial currents -- which are the quantities actually used in the sample calculations are summarized below -- are obtained straightforwardly from Eqs. (29) and (31).

DISCUSSION

Starting from the three-dimensional transport equation and utilizing three spatial scales in an asymptotic development of a reactor homogenization theory -- by introducing the spatial scales for the three physically relevant geometric units in the reactor: the unit lattice cell, the unit fuel bundle and the overall reactor -- we have advanced a homogenization theory based on systematic mathematical developments so that the cell and bundle homogenization schemes have been developed systematically and simultaneously. This work is an extension of previous analyses of unit fuel lattices homogenization carried out using two spatial scales⁵⁻⁷. In fact, the results we obtain at the ϵ^2 order, in the form of cell homogenized diffusion equation and homogenized parameters, are the same as reported in Ref. 7: the cell homogenized diffusion equation has the drift and source (or sink) terms and cell homogenized diffusion coefficients and cross sections for the unit fuel cell have been bilinearly weighted by the unit cell fundamental eigenfunction and its adjoint⁷.

Motivated by the appropriate size of fuel bundle for nodal analysis, an extension of asymptotic analysis to near periodic fuel bundles was reported by Chiang⁸. He started with conventional multigroup diffusion equation for fuel bundle to develop the bundle homogenized diffusion equation for the reactor

core. [The analysis in Ref. 8 is greatly simplified due to an algebraic error which resulted in the loss of the cross terms (of order ϵ) that should appear from the second derivative term in the diffusion equation.] This approach had the disadvantage that the final eigenvalue obtained is an approximation to the diffusion eigenvalue. Moreover, the validity of using the conventional diffusion equation is questionable as it does not include the drift and source terms -- which very naturally appear in our systematic development from the transport equation -- in the homogenized diffusion equation for the unit fuel bundle.

Our bundle homogenized global diffusion equation for the reactor results from the successive application of the Fredholm alternative theorem on the ϵ^4 order equation. First, the application of the Fredholm alternative for the operator F (defined in Eq. (3)) yields an inhomogeneous equation which has the same diffusion operator as one obtained at the ϵ^2 order. Hence, another application of Fredholm alternative, now for the diffusion operator (L in Eq. (I-C-1)) results in the bundle-homogenized global diffusion equation for the reactor. As was the case in the bundle diffusion equation obtained at the ϵ^2 order, there are drift and source terms in this final diffusion equation. These terms have been known to exist in the diffusion equation in non-periodic media.^{5,6,7}

The bundle-homogenized diffusion coefficient obtained is of the form $\underline{D}_b = \underline{D}_b^0 + \underline{D}_b^1 + \underline{D}_b^2 + \underline{D}_b^3$, where $\underline{D}_b^0$ is the diffusion tensor obtained by bilinearly averaging the cell homogenized diffusion tensor elements with the fundamental forward and adjoint eigenfunctions for the unit fuel bundle. $\underline{D}_b^1$, $\underline{D}_b^2$ and $\underline{D}_b^3$ are the terms that account for the non-periodic nature of the fuel lattices as well as bundles. Similarly, the homogenized cross sections are obtained by bilinearly weighting the cell homogenized cross sections with the unit fuel bundle fundamental eigenfunction and its adjoint.

As discussed in the previous section, the discontinuity or jump conditions at the cell interfaces for the solution of the cell-homogenized bundle diffusion equation and at the bundle interfaces for the solution of the bundle-homogenized global diffusion equation follow from the continuity of the angular flux. Since the fundamental cell eigenfunction for one cell is different from another because of the deviation of nuclear parameters from exact periodicity, Eq. (30) gives rise to the finite jump condition for A_0 . For the bundle-homogenized diffusion equation, the fact that the fundamental eigenfunction in one bundle is different from the neighboring bundle eigenfunction due to non-periodic bundles, leads to the finite jump condition for a_0 on the bundle interfaces for non-periodic arrays. These jump conditions are analogous to, but different from, the ad hoc discontinuity conditions proposed earlier by Kobke³ and later extended by Smith⁴.

The method developed here also makes de-homogenization possible. In fact no extra work is needed to obtain the detailed flux distribution inside the fuel bundles and lattice cells. The interior bundle and cell fluxes can be reconstructed using Eqs. (4) and (13). This 'de-homogenization' step naturally yields in the leading order angular flux solution to the original transport equation. Thus, in addition to yielding a fourth-order accurate approximation to the exact transport theory eigenvalue $1/k_{\text{eff}}$, the homogenization theory also yields the transport theory angular flux to leading order.

NUMERICAL RESULTS

Several test problems, in which the multiple-scales homogenization theory was incorporated into nodal diffusion calculations, have been studied. These calculations were done using the nodal Green's function method (NGFM), with

coarse-mesh rebalancing and asymptotic source extrapolation, for the diffusion calculations. The discrete nodal transport method (DNTM), in the S-16 approximation, also with coarse-mesh rebalancing and asymptotic source extrapolation, was used for both the lattice cell homogenization calculations and the global heterogeneous system transport calculations of the reference solutions. Results for three of these problems, one extremely simple, are summarized here. The simple first problem is reported merely to demonstrate that, consistent with the homogenization theory, as the system is made larger and the expansion parameter becomes smaller the homogenized diffusion theory results better approximate the exact transport theory results. This simple system was comprised of an exactly periodic one-dimensional array of lattice cells of one type only; hence, it really is an example of the special case in which only two, rather than three, spatial scales are present.⁵⁻⁷ The cell was comprised of a 1.2 cm central fuel region flanked by two 0.2 cm water regions. Since it was symmetric, reflective cell transport boundary conditions are equivalent to periodic boundary conditions, and the former were used in the 16-equal-node DNTM transport calculations of the cell eigenvalue $1/k_0$, the cell eigenfunction $\psi_0^{(0)}(x, \mu)$ and the solution to the inhomogeneous cell transport equation $f(x, \mu)$ used in construction of the cell-homogenized diffusion coefficient. Further, since the cell was symmetric, the cell interface discontinuity factors were unity. That is, the global diffusion theory flux and current are continuous in this special case. The results of the global reactor NGFM diffusion calculations, done using one node per cell, for a sequence of symmetric systems comprised of 15, 20, 25 and 30 lattice cells between the symmetry plane and boundary are summarized in Table 1, in which they are compared with DNTM global transport calculations done using 16 nodes per cell. Clearly as the system becomes larger, and the expansion parameter ϵ

used in the asymptotic development of the homogenization theory becomes smaller, the homogenized nodal diffusion theory results more accurately approximate the exact nodal transport theory result.

Table 1. Comparisons of Cell-Homogenized Nodal Diffusion Calculations with Global Nodal Transport Calculations for Test Problem No. 1^a

No ^b of Lattice Cells	Diffusion Calculation ^c		Transport Calculation ^d		$\Delta k_{\text{eff}}/k_{\text{eff}}$ (%)
	k_{eff}	CPU(s) ^e	k_{eff}	CPU(s)	
15	0.94220898	2.76	0.94165241	42.20	0.0591
20	0.94279900	2.82	0.94248000	76.60	0.0339
25	0.94307424	2.90	0.94286785	136.27	0.0219
30	0.94322446	2.96	0.94308011	244.59	0.0153

^aCross sections (isotropic scatt.): Fuel -- $\nu\Sigma_f = 0.4975$; $\Sigma_s = 0.5800$; $\Sigma_a = 0.5200$. Water -- $\Sigma_s = 3.4500$; $\Sigma_a = 0.0220$. Homogenized --

$\nu\Sigma_f = 0.3751567775$; $\bar{D} = 0.1370111251$; $\bar{\Sigma}_a = 0.3975935339$.

^bBetween symmetry plane and boundary.

^cConvergence criteria on scalar fluxes: 10^{-9} .

^dConvergence criteria on scalar fluxes: $\psi_0^{(o)}$ (used as source in calc. of $f(x, \mu)$) - 10^{-11} ; $f(x, \mu)$ - 10^{-9} ; diff. calc. - 10^{-9} .

^eIncludes cell transp. calc. and calc. of homogenized diff. th. param.

The second test problem was for a system made up of three near-periodic bundles in slab geometry: a fresh fuel bundle located in the inner-most region adjacent to the plane of symmetry, a control bundle in the second region with much higher absorption in the water, and a partially depleted bundle in the outer region representing one from a previous cycle shuffled to that position. Each was comprised of five exactly periodic symmetric cells with a 0.8 cm central fuel region and a 0.4 cm water region on each side.

The cell transport eigenvalue $1/k_0$, the cell eigenfunction $\psi_0^{(o)}(x, \mu)$ and $f(x, \mu)$ were computed for each type cell using the DNTM in the S-16 approximation with 8 equal nodes in a cell. Since each different bundle in this problem contains only one type cell there are no cell discontinuity factors within a bundle, and the fundamental eigenfunction of the cell-homogenized bundle diffusion equation with periodic boundary conditions is a simple constant. Hence, this second test problem also is a special case, of the general homogenization theory, in which real discontinuity factors occur only at bundle interfaces, and are due only to the difference between the surface values of the two different cell eigenfunctions on the opposite sides of the bundle interface. The bundle-homogenized global diffusion equation then follows immediately from the cell homogenization. This global diffusion equation was solved using the NGFM with one node per cell, i.e. fifteen nodes, both without and with the flux and current discontinuity factors, which are the same for this special case due to the symmetry of the cells and bundles. The resulting values of k_{eff} and the bundle powers are compared in Table 2 with those of the exact transport global calculation done using the DNTM in the S-16 approximation with 8 nodes per cell -- a total of 120 nodes.

Table 2. Comparison of Homogenized Nodal Diffusion Calculations
with Nodal Transport Calculation for Test Problem No. 2^a

Calculation	k_{eff} (Error) ^b	Power in Bundle 1 (Error) ^{b,c}	Power in Bundle 2 (Error) ^{b,c}	Power in Bundle 3 (Error) ^{b,c}
Transport ^d	0.95267431	0.84082021	0.14629769	0.01288210
Diffusion ^e w/o Disc. Factors	0.95382244 (0.00114813)	0.85391153 (0.01309132)	0.13690219 (-0.00939550)	0.00918628 (-0.00369581)
Diffusion ^e w/ Disc. Factors ^f	0.95322648 (0.00055217)	0.84400114 (0.00318093)	0.14690544 (0.00060774)	0.00909342 (-0.00378867)
Fine-Mesh Diffusion ^d	0.95101362 (-0.00166069)	0.82570269 (-0.01511752)	0.15769090 (0.01139320)	0.01660641 (0.00372432)

^aCross sections (isotropic scatt.): Bundle 1: Fuel -- $\nu\Sigma_f = 0.5500$;
 $\Sigma_s = 0.5500$; $\Sigma_a = 0.5500$. Water -- $\Sigma_s = 3.4500$; $\Sigma_a = 0.0220$.
Homogenized -- $\nu\Sigma_f = 0.2822208616$; $\bar{D} = 0.1205289564$; $\bar{\Sigma}_a = 0.2932172444$.
Bundle 2: Fuel -- $\nu\Sigma_f = 0.5500$; $\Sigma_s = 0.5500$; $\Sigma_a = 0.5500$.
Water -- $\Sigma_s = 3.4500$; $\Sigma_a = 0.0620$. Homogenized -- $\nu\Sigma_f = 0.2949153901$;
 $\bar{D} = 0.1206996200$; $\bar{\Sigma}_a = 0.3258378029$.
Bundle 3: Fuel -- $\nu\Sigma_f = 0.5400$; $\Sigma_s = 0.5500$; $\Sigma_a = 0.5600$.
Water -- $\Sigma_s = 3.4500$; $\Sigma_a = 0.0220$. Homogenized -- $\nu\Sigma_f = 0.2770897784$;
 $\bar{D} = 0.1201555640$; $\bar{\Sigma}_a = 0.2983487512$.

^bError with respect to transport theory value.

^cError in bundle power as a fraction of total power (normalized 1.0).

^dConvergence criteria on scalar fluxes: 10^{-11}

^eConvergence criteria on scalar fluxes: $\psi_o^{(o)}$ (used as source in calc. of
 $f(x,\mu) - 10^{-13}$; $f(x,\mu) - 10^{-11}$; diff. calc. - 10^{-11} .

^fDiscontinuity factors(+/-): Bundle 2/1 - 0.96311735; Bundle 3/2 -
1.03830159

Table 2 shows that the systematically homogenized nodal diffusion calculation rather accurately recovers the exact transport theory values for k_{eff} and the bundle powers, even when the discontinuity factors are omitted. It also shows that for this problem the small error in k_{eff} is further decreased by about a factor of two when the discontinuity factors are included, and the errors in the powers of the two higher power fuel assemblies also decrease significantly when they are included.

A third test problem that was studied was analogous to the second with identical geometry, but with less absorption in the control bundle and with a water reflector equal in width to one bundle. The homogenization theory easily extends to this case since the reflector is homogeneous and therefore trivially periodic. The results obtained for that problem, both with and without the reflector, were similar both qualitatively and quantitatively to those just summarized for Problem No. 2; however, because of the reflector, the cell power and flux distributions are more representative of those that occur in power reactors. The computed cell power distributions are shown in Fig. 1 for: the homogenized 20-node diffusion calculation without discontinuity factors; the homogenized 20-node diffusion calculation with discontinuity factors; the fine-mesh 160-node global transport calculation; and the fine-mesh 160-node global diffusion calculation. The L_1 errors (average absolute value of the errors) of the cell powers as a fraction of the total power were 0.002566 and 0.001655 respectively for the calculations without and with discontinuity factors, and the corresponding maximum errors in the cell powers were 0.007238 and 0.005165. For the fine-mesh nodal diffusion calculation the L_1 and maximum errors were 0.001874 and -0.005183. Finally, the detailed reconstructed or 'de-homogenized' fluxes -- based on the product of the global nodal diffusion solution, the bundle nodal diffusion solution (a constant for this problem) and the cell nodal transport solution, as given by the leading order solution in the homogenization theory -- are compared in Fig. 2 with the detailed scalar fluxes from the whole-system nodal transport theory reference solution, and with the fine-mesh whole-system nodal diffusion computed flux. The flux reconstructed from the homogenized 20-node diffusion calculation with discontinuity factors agrees better with that from the 160-node transport calculation than does that reconstructed from the calculation done without

Figure 1. Cell power distributions for Test Problem No. 3. Cross sections (isotropic scatt.): Bundle 1: Fuel -- $\nu\Sigma_f = 0.5500$; $\Sigma_s = 0.5500$; $\Sigma_a = 0.5500$. Water -- $\Sigma_s = 3.4500$; $\Sigma_a = 0.0220$. Homogenized -- $\nu\Sigma_f = 0.2822208616$; $D = 0.1205209564$; $\bar{\Sigma}_a = 0.2932172444$. Bundle 2: Fuel -- $\nu\Sigma_f = 0.5500$; $\Sigma_s = 0.5500$; $\Sigma_a = 0.5500$. Water -- $\Sigma_s = 3.4800$; $\Sigma_a = 0.0300$. Homogenized -- $\nu\Sigma_f = 0.2848047936$; $D = 0.1205804605$; $\bar{\Sigma}_a = 0.2997956999$. Bundle 3: Fuel -- $\nu\Sigma_f = 0.5470$; $\Sigma_s = 0.5500$; $\Sigma_a = 0.5500$. Water -- $\Sigma_s = 3.4500$; $\Sigma_a = 0.0220$. Homogenized -- $\nu\Sigma_f = 0.2810919781$; $D = 0.1205209564$; $\bar{\Sigma}_a = 0.2932172444$.

Figure 2. Comparison of reconstructed fluxes with the full fine mesh transport theory computed fluxes and with the full fine mesh diffusion theory computed fluxes for Test Problem No. 3.

discontinuity factors, and both agree better with it than does that from the 160-node fine-mesh diffusion calculation.

Several other test problems with 3, 4, 5 and 6 bundles have been studied. In all cases the errors in k_{eff} were small, and they decreased when the discontinuity factors were introduced. However, in some problems the small errors in the bundle powers and cell powers increased slightly when the discontinuity factors were used.

SUMMARY OF PART I

A self-consistent and systematic lattice-cell and fuel-bundle homogenization theory has been developed by introducing three spatial scales in an asymptotic expansion of the solution to the transport equation. The resulting homogenized diffusion coefficients and cross sections for the cell-homogenized bundle diffusion equation and bundle-homogenized global diffusion equation are bilinearly weighted by forward and adjoint fluxes in contrast to conventional flux weighted parameters. The development provides a practical homogenization theory for incorporation into nodal diffusion methods for reactor calculations. The final reactor diffusion calculation yields the exact transport equation angular flux to lowest order and the exact transport equation eigenvalue $1/k_{eff}$ to fourth order in the small parameter. Nodal interface jump conditions on the flux and current -- to be used in the solution of homogenized diffusion equation for the fuel bundles and the reactor -- have been obtained. The results also provide a flux reconstruction or 'de-homogenization' procedure by which cell interior and bundle interior fluxes can be easily reconstructed. Test problems studied demonstrate the accuracy of the homogenization theory and its compatibility with nodal transport and nodal diffusion methods.

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Appendix I-A

$$\begin{aligned}
 \gamma(\underline{n}, \underline{\zeta}) = G\theta_o^{(o)} = & \langle \psi_o^{(o)\dagger}, \hat{\Omega} \cdot \nabla_{\underline{n}} (f_1 \frac{\partial^2 \theta_o^{(o)}}{\partial \eta_1^2} + g_1 \frac{\partial^2 \theta_o^{(o)}}{\partial \eta_1 \partial \eta_2} + f_2 \frac{\partial^2 \theta_o^{(o)}}{\partial \eta_2^2} \\
 & + p_1 \frac{\partial \theta_o^{(o)}}{\partial \eta_1} + p_2 \frac{\partial \theta_o^{(o)}}{\partial \eta_2} + z\theta_o^{(o)} - f \frac{\partial \theta_o^{(o)}}{\partial \zeta_1} - g \frac{\partial \theta_o^{(o)}}{\partial \zeta_2} - h \frac{\partial \theta_o^{(o)}}{\partial \zeta_3}) \rangle_c \\
 & + \frac{1}{k_{1,\underline{\zeta}}^2} \langle \psi_o^{(o)\dagger}, \nu_{\underline{f}} (\bar{f} \frac{\partial^2 \theta_o^{(o)}}{\partial \eta_1^2} + \bar{g} \frac{\partial^2 \theta_o^{(o)}}{\partial \eta_1 \partial \eta_2} + \bar{f} \frac{\partial^2 \theta_o^{(o)}}{\partial \eta_2^2} + \bar{p} \frac{\partial \theta_o^{(o)}}{\partial \eta_1} \\
 & + \bar{p}_2 \frac{\partial \theta_o^{(o)}}{\partial \eta_2} + \bar{z}\theta_o^{(o)} - \bar{f} \frac{\partial \theta_o^{(o)}}{\partial \zeta_1} - \bar{g} \frac{\partial \theta_o^{(o)}}{\partial \zeta_2}) \rangle_c \\
 & + \frac{1}{k_{2,0}^2} \langle \psi_o^{(o)\dagger}, \nu_{\sigma f} (\bar{f} \frac{\partial \theta_o^{(o)}}{\partial \eta_1} + \bar{g} \frac{\partial \theta_o^{(o)}}{\partial \eta_2} + (\bar{f}' + \bar{g}' - \bar{q})\theta_o^{(o)}) \rangle_c \\
 & - \langle \psi_o^{(o)\dagger}, \hat{\Omega} \cdot \nabla_{\underline{\zeta}} (f \frac{\partial \theta_o^{(o)}}{\partial \eta_1} + g \frac{\partial \theta_o^{(o)}}{\partial \eta_2} + (f' + g' - q)\theta_o^{(o)}) \rangle_c \\
 & - k \frac{1}{3} \langle \psi_o^{(o)\dagger}, \frac{1}{f} \bar{\psi}_o^{(o)} \theta_o^{(o)} \rangle_c
 \end{aligned} \tag{I-A-1}$$

and

$$\begin{aligned}
 \omega_i(\underline{n}, \underline{\zeta}) = w_i \theta_o^{(o)} = & \langle \psi_o^{(o)\dagger}, \hat{\Omega} \cdot \nabla_{\underline{n}} (\ell_i \theta_o^{(o)}) \rangle_c \\
 & + \langle \psi_o^{(o)\dagger}, \Omega_i (f \frac{\partial \theta_o^{(o)}}{\partial \eta_1} + g \frac{\partial \theta_o^{(o)}}{\partial \eta_2} + (f' + g' - q)\theta_o^{(o)}) \rangle_c \\
 & - \langle \psi_o^{(o)\dagger}, \frac{1}{k_{1,\underline{\zeta}}} \nu_{\sigma f} \bar{\ell}_i \theta_o^{(o)} \rangle_c ; \quad i=1,2
 \end{aligned} \tag{I-A-2}$$

and $\underline{\ell} = [f, g, h]$.

Appendix I-B

$$\begin{aligned}
 FH(\xi_1, \xi_2, \eta, \zeta, \hat{\Omega}, A_o) = & - \hat{\Omega} \cdot \nabla_{\eta} (f_1 \frac{\partial^2 A_o}{\partial \eta_1^2} + g_1 \frac{\partial^2 A_o}{\partial \eta_1 \partial \eta_2} + f_2 \frac{\partial^2 A_o}{\partial \eta_2^2} \\
 & + P_1 \frac{\partial A_o}{\partial \eta_1} + P_2 \frac{\partial A_o}{\partial \eta_2} + Z A_o) + \hat{\Omega} \cdot \nabla_{\zeta} (f \frac{\partial A_o}{\partial \zeta_1} + g \frac{\partial A_o}{\partial \zeta_2} + h \frac{\partial A_o}{\partial \zeta_3}) \\
 & + \hat{\Omega} \cdot \nabla_{\zeta} (f \frac{\partial A_o}{\partial \eta_1} + g \frac{\partial A_o}{\partial \eta_2} + (f' + g' - q) A_o) \\
 & + \frac{1}{k_1^{\eta, \zeta}} \nu \sigma_f (\bar{f}_1 \frac{\partial^2 A_o}{\partial \eta_1^2} + \bar{g}_1 \frac{\partial^2 A_o}{\partial \eta_1 \partial \eta_2} + \bar{f}_2 \frac{\partial^2 A_o}{\partial \eta_2^2} + \bar{P}_1 \frac{\partial A_o}{\partial \eta_1} \\
 & + \bar{P}_2 \frac{\partial A_o}{\partial \eta_2} + \bar{Z} A_o - \bar{f} \frac{\partial A_o}{\partial \zeta_1} - \bar{g} \frac{\partial A_o}{\partial \zeta_2}) \\
 & - \frac{1}{k_2^{\eta, \zeta}} \nu \sigma_f (\bar{f} \frac{\partial A_o}{\partial \eta_1} + \bar{g} \frac{\partial A_o}{\partial \eta_2} + (\bar{f}' + \bar{g}' - \bar{q}) A_o) + \frac{1}{k_3^{\zeta}} \nu \sigma_f \bar{\psi}_o^{(o)} A_o
 \end{aligned}
 \tag{I-B-1}$$

The solution for H is

$$\begin{aligned}
 H(\xi_1, \xi_2, \eta, \zeta, \hat{\Omega}, A_o) = & - y(\xi_1, \xi_2, \eta, \zeta, \hat{\Omega}) a_o(\zeta) \\
 & + \beta(\xi_1, \xi_2, \eta, \zeta, \hat{\Omega}) \cdot \nabla_{\zeta} a_o
 \end{aligned}$$

where y and β satisfy

$$\begin{aligned}
 Fy(\xi_1, \xi_2, \eta, \zeta, \hat{\Omega}) = & \hat{\Omega} \cdot \nabla_{\eta} (f_1 \frac{\partial^2 \theta_o^{(o)}}{\partial \eta_1^2} + g_1 \frac{\partial^2 \theta_o^{(o)}}{\partial \eta_1 \partial \eta_2} + f_2 \frac{\partial^2 \theta_o^{(o)}}{\partial \eta_2^2} \\
 & + P_1 \frac{\partial \theta_o^{(o)}}{\partial \eta_1} + P_2 \frac{\partial \theta_o^{(o)}}{\partial \eta_2} + Z \theta_o^{(o)} - f \frac{\partial \theta_o^{(o)}}{\partial \zeta_1} - g \frac{\partial \theta_o^{(o)}}{\partial \zeta_2} - h \frac{\partial \theta_o^{(o)}}{\partial \zeta_3})
 \end{aligned}$$

$$\begin{aligned}
& - \hat{\Omega} \cdot \nabla_{\xi} \left(f \frac{\partial \theta_o^{(o)}}{\partial \eta_1} + g \frac{\partial \theta_o^{(o)}}{\partial \eta_2} + (f' + g' - q) \theta_o^{(o)} \right) \\
& - \frac{1}{k_1^{\eta, \xi}} \nu_{\sigma f} (\bar{f}_1 \frac{\partial^2 \theta_o^{(o)}}{\partial \eta_1^2} + \bar{g}_1 \frac{\partial^2 \theta_o^{(o)}}{\partial \eta_1 \partial \eta_2} + \bar{f}_2 \frac{\partial^2 \theta_o^{(o)}}{\partial \eta_2^2} + \bar{p}_1 \frac{\partial \theta_o^{(o)}}{\partial \eta_1} \\
& + \bar{p}_2 \frac{\partial \theta_o^{(o)}}{\partial \eta_2} + \bar{z} \theta_o^{(o)} - \bar{f} \frac{\partial \theta_o^{(o)}}{\partial \xi_1} - \bar{g} \frac{\partial \theta_o^{(o)}}{\partial \xi_2}) \\
& + \frac{1}{k_{2,0}^{\eta, \xi}} \nu_{\sigma f} (\bar{f} \frac{\partial \theta_o^{(o)}}{\partial \eta_1} + \bar{g} \frac{\partial \theta_o^{(o)}}{\partial \eta_2} + (\bar{f}' + \bar{g}' - \bar{q}) \theta_o^{(o)}) \\
& - \frac{1}{k_3^{\xi}} \nu_{\sigma f} \bar{\psi}_o^{(o)} \theta_o^{(o)}
\end{aligned}$$

and

$$\begin{aligned}
F\beta_i(\xi_1, \xi_2, \eta, \xi, \hat{\Omega}) - \hat{\Omega} \cdot \nabla_{\eta} (\ell_i \theta_o^{(o)}) + \Omega_i \left(f \frac{\partial \theta_o^{(o)}}{\partial \eta_1} + g \frac{\partial \theta_o^{(o)}}{\partial \eta_2} \right. \\
\left. + (f' + g' - q) \theta_o^{(o)} \right) - \frac{1}{k_1^{\eta, \xi}} \nu_{\sigma f} \bar{\ell}_i \theta_o^{(o)} ; i = 1, 2
\end{aligned}$$

Appendix I-C

$$L A_2(\underline{n}, \underline{\zeta}) = \langle \psi_o^{(o)\dagger}, \hat{\Omega} \cdot \nabla_{\underline{n}} (f_1 \frac{\partial^2 A_1}{\partial \eta_1^2} + g_1 \frac{\partial^2 A_1}{\partial \eta_1 \partial \eta_2} + f_2 \frac{\partial^2 A_1}{\partial \eta_2^2} + p_1 \frac{\partial A_1}{\partial \eta_2} + p_2 \frac{\partial A_1}{\partial \eta_1} - f \frac{\partial A_1}{\partial \eta_2} - g_1 \frac{\partial A_1}{\partial \zeta_3} - h \frac{\partial A_1}{\partial \zeta} \partial \zeta) \rangle_c$$

$$- \langle \psi_o^{(o)\dagger}, \hat{\Omega} \cdot \nabla_{\underline{\zeta}} (f \frac{\partial A_1}{\partial \eta_1} + g \frac{\partial A_1}{\partial \eta_2} + (f' + g' - q) A_1) \rangle_c$$

$$- \frac{1}{k_1^{\underline{n}, \underline{\zeta}}} \langle \psi_o^{(o)\dagger}, \nu_{\sigma f} (\bar{f}_1 \frac{\partial^2 A_1}{\partial \eta_1^2} + \bar{g}_1 \frac{\partial^2 A_1}{\partial \eta_1 \partial \eta_2} + \bar{f}_2 \frac{\partial^2 A_1}{\partial \eta_2^2} + \bar{p}_1 \frac{\partial A_1}{\partial \eta_1} + \bar{p}_2 \frac{\partial A_1}{\partial \eta_2} + \bar{z} A_1 - \bar{f} \frac{\partial A_1}{\partial \zeta_1} - \bar{g} \frac{\partial A_1}{\partial \zeta_2}) \rangle_c$$

$$+ \frac{1}{k_{2,0}^{\underline{n}, \underline{\zeta}}} \langle \psi_o^{(o)\dagger}, \nu_{\sigma f} (\bar{f} \frac{\partial A_1}{\partial \eta_1} + \bar{g} \frac{\partial A_1}{\partial \eta_2} + (\bar{f}' + \bar{g}' - \bar{q}) A_1) \rangle_c$$

$$- \frac{1}{k_3^{\underline{\zeta}}} \langle \psi_o^{(o)\dagger}, \nu_{\sigma f} \bar{\psi}_o^{(o)} A_1 \rangle_c$$

$$+ \langle \psi_o^{(o)\dagger}, \hat{\Omega} \cdot \nabla_{\underline{n}} H(\xi_1, \xi_2, \underline{n}, \underline{\zeta}, \hat{\Omega}, A_o) \rangle_c$$

$$+ \langle \psi_o^{(o)\dagger}, \hat{\Omega} \cdot \nabla_{\underline{\zeta}} (f_1 \frac{\partial^2 A_o}{\partial \eta_1^2} + g_1 \frac{\partial^2 A_o}{\partial \eta_1 \partial \eta_2} + f_2 \frac{\partial^2 A_o}{\partial \eta_2^2} + p_1 \frac{\partial A_o}{\partial \eta_1} + p_2 \frac{\partial A_o}{\partial \eta_2} + z A_o - f \frac{\partial A_o}{\partial \zeta_1} - g \frac{\partial A_o}{\partial \zeta_2} - h \frac{\partial A_o}{\partial \zeta_3}) \rangle_c$$

$$- \frac{1}{k_1^{\underline{n}, \underline{\zeta}}} \langle \psi_o^{(o)\dagger}, \nu_{\sigma f} \bar{H}(\xi_1, \xi_2, \underline{n}, \underline{\zeta}, \hat{\Omega}, A_o) \rangle_c$$

$$\begin{aligned}
& - \frac{1}{k_{2,0}^{\eta, \zeta}} \langle \psi_o^{(o)\dagger}, \nu_{\sigma_f} (\bar{f}_1 \frac{\partial^2 A_o}{\partial \eta_1^2} + \bar{g}_1 \frac{\partial^2 A_o}{\partial \eta_1 \partial \eta_2} + \bar{f}_2 \frac{\partial^2 A_o}{\partial \eta_2^2} \\
& \quad + \bar{p}_1 \frac{\partial A_o}{\partial \eta_1} + \bar{p}_2 \frac{\partial A_o}{\partial \eta_2} + \bar{z} A_o - \bar{f} \frac{\partial A_o}{\partial \zeta_1} - \bar{g} \frac{\partial A_o}{\partial \zeta_2}) \rangle_c \\
& + \frac{1}{k_3^{\zeta}} \langle \psi_o^{(o)\dagger}, \nu_{\sigma_f} (\bar{f} \frac{\partial A_o}{\partial \eta_1} + \bar{g} \frac{\partial A_o}{\partial \eta_2} + (\bar{f}' + \bar{g}' - \bar{q}) A_o) \rangle_c \\
& - \frac{1}{k_4} \langle \psi_o^{(o)\dagger}, \nu_{\sigma_f} \bar{\psi}_o^{(o)} A_o \rangle_c
\end{aligned}$$

(I-C-1)

Appendix I-D

$$\begin{aligned}
 & (\nabla_{\underline{\zeta}} \cdot \underline{D}_b^0 \cdot \nabla_{\underline{\zeta}} a_o - \nabla_{\underline{\zeta}} \cdot (\underline{D}_b^1 + \underline{D}_b^2) \cdot \nabla_{\underline{\zeta}} a_o) \\
 & + (\langle \theta_o^{(o)\dagger}, \langle \psi_o^{(o)\dagger}, \hat{\Omega} \cdot \nabla_{\underline{\eta}} y \rangle_c \rangle_b - \langle \theta_o^{(o)\dagger}, \frac{1}{k_{1,\underline{\zeta}}^{\underline{\eta}}} \langle \psi_o^{(o)\dagger}, \nu \sigma_{\underline{f}} \bar{y} \rangle_c \rangle_b \\
 & + \langle \theta_o^{(o)\dagger}, \frac{1}{k_{2,0}^{\underline{\eta}, \underline{\zeta}}} \langle \psi_o^{(o)\dagger}, \nu \sigma_{\underline{f}} (\bar{f}_1 \frac{\partial^2 \theta_o^{(o)}}{\partial \eta_1^2} + \bar{g}_1 \frac{\partial^2 \theta_o^{(o)}}{\partial \eta_1 \partial \eta_2} + \bar{f}_2 \frac{\partial^2 \theta_o^{(o)}}{\partial \eta_2^2} \\
 & + \bar{p}_1 \frac{\partial \theta_o^{(o)}}{\partial \eta_1} + \bar{p}_2 \frac{\partial \theta_o^{(o)}}{\partial \eta_2} + \bar{z} \theta_o^{(o)} - \bar{f} \frac{\partial \theta_o^{(o)}}{\partial \zeta_1} - \bar{g} \frac{\partial \theta_o^{(o)}}{\partial \zeta_2}) \rangle_c \rangle_b \\
 & - \langle \theta_o^{(o)\dagger}, \frac{1}{k_{3,\underline{\zeta}}^{\underline{\eta}}} \langle \psi_o^{(o)\dagger}, \nu \sigma_{\underline{f}} (\bar{f} \frac{\partial \theta_o^{(o)}}{\partial \eta_1} + \bar{g} \frac{\partial \theta_o^{(o)}}{\partial \eta_2} + (\bar{f}' + \bar{g}' - \bar{q}) \theta_o^{(o)}) \rangle_c \rangle_b \\
 & + \langle \theta_o^{(o)\dagger}, \frac{1}{k_4} \langle \psi_o^{(o)\dagger}, \nu \sigma_{\underline{f}} \bar{\psi}_o^{(o)} \theta_o^{(o)} \rangle_c \rangle_b - \langle \theta_o^{(o)\dagger}, \gamma' \rangle_b) a_o(\underline{\zeta}) \\
 & + (- \langle \theta_o^{(o)\dagger}, \langle \psi_o^{(o)\dagger}, \hat{\Omega} \cdot \nabla_{\underline{\eta}} \underline{\beta} \rangle_c \rangle_b - \langle \theta_o^{(o)\dagger}, \langle \psi_o^{(o)\dagger}, \hat{\Omega} (f_1 \frac{\partial^2 \theta_o^{(o)}}{\partial \eta_1^2} \\
 & + g_1 \frac{\partial^2 \theta_o^{(o)}}{\partial \eta_1 \partial \eta_2} + f_2 \frac{\partial^2 \theta_o^{(o)}}{\partial \eta_2^2} + p_1 \frac{\partial \theta_o^{(o)}}{\partial \eta_1} + p_2 \frac{\partial \theta_o^{(o)}}{\partial \eta_2} + z \theta_o^{(o)} - f \frac{\partial \theta_o^{(o)}}{\partial \zeta_1} \\
 & - g \frac{\partial \theta_o^{(o)}}{\partial \zeta_2} - h \frac{\partial \theta_o^{(o)}}{\partial \zeta_3}) \rangle_c \rangle_b - \Omega - \langle \theta_o^{(o)\dagger}, \langle \hat{\Omega} \cdot \nabla_{\underline{f}} \psi_o^{(o)\dagger}, \underline{\ell} \rangle_c \theta_o^{(o)} \rangle_b \\
 & + \langle \theta_o^{(o)\dagger}, \frac{1}{k_{1,\underline{\zeta}}^{\underline{\eta}}} \langle \psi_o^{(o)\dagger}, \nu \sigma_{\underline{f}} \bar{\underline{\beta}} \rangle_c \rangle_b + \langle \theta_o^{(o)\dagger}, \underline{\omega}' \rangle_b + \underline{x} + \underline{y} \\
 & - \langle \theta_o^{(o)\dagger}, \frac{1}{k_{2,0}^{\underline{\eta}, \underline{\zeta}}} \langle \psi_o^{(o)\dagger}, \nu \sigma_{\underline{f}} \underline{\ell} \rangle_c \theta_o^{(o)} \rangle_b + \langle \theta_o^{(o)\dagger}, \underline{\gamma}'' \rangle_b) \cdot \nabla_{\underline{\zeta}} a_o \\
 & + \nabla_{\underline{\zeta}} \cdot \langle \theta_o^{(o)\dagger}, \underline{w} \rangle a_1 = 0
 \end{aligned}
 \tag{I-D-1}$$

where $\underline{\omega}' = [W_1 v(\underline{n}, \underline{\zeta}), W_2 v(\underline{n}, \underline{\zeta})]$; $\gamma' = G v(\underline{n}, \underline{\zeta})$;

$\underline{\gamma}'' = G \underline{\gamma}(\underline{n}, \underline{\zeta})$; and $Q_i = \langle \frac{\partial}{\partial \zeta_i} \theta^{(o)\dagger}, \langle \psi_o^{(o)\dagger}, \Omega_i \ell_i \rangle_c \theta_o^{(o)} \rangle_b$, $i = 1, 2, 3$;

$X_i = \nabla_{\zeta} \cdot \langle \theta_o^{(o)\dagger}, \langle \psi_o^{(o)\dagger}, \hat{A} \cdot \nabla_{\underline{n}} (\underline{\ell} r_i) - \frac{1}{k_1} \nu \sigma_f \bar{\ell} r_i \rangle_c \theta_o^{(o)} \rangle_b$, $i = 1, 2$;

$Y_i = \nabla_{\zeta} \cdot \langle \theta_o^{(o)\dagger}, \langle \psi_o^{(o)\dagger}, \hat{A} (f \frac{\partial}{\partial \eta_1} + g \frac{\partial}{\partial \eta_2} + f' + g' - q) r_i \rangle_c \theta_o^{(o)} \rangle_b$, $i = 1, 2$;

and the operator G is given by Eq. (I-A-1), W_i , $i = 1, 2$; Ω_i , $i = 1, 2$; is given by Eq. (I-A-2)

and R is given by Eq. (17).

PART II: APPLICATIONS OF A SYSTEMATIC HOMOGENIZATION THEORY FOR NODAL DIFFUSION METHODS

In Part I, we have developed, for use with nodal diffusion methods, a self-consistent and systematic lattice-cell and fuel-bundle homogenization theory based on a multiple-spatial-scales asymptotic expansion of the transport equation in the ratio of the mean free path to the reactor characteristic dimension.¹ The mathematical development leads naturally to self-consistent analytical expressions for homogenized diffusion coefficients and cross sections, and flux discontinuity factors, to be used in nodal diffusion calculations. The expressions for the homogenized nuclear parameters that follow from the systematic homogenization theory (SHT) are different from those for the traditional flux and volume weighted (FVW) parameters. The computational framework that results from the SHT was applied in Part I (and in Ref. 1) to numerical examples that included both lattice-cell and fuel-bundle homogenization -- but only for somewhat simple one-dimensional systems.¹ Here, in Part II of this report, we summarize results of the application of these homogenization procedures to nodal diffusion calculations for realistic 2-D pressurized water reactor (PWR) models. They show, for the problems studied, that coarse-mesh nodal diffusion calculations, done using assembly size nodes and the homogenized diffusion coefficients and cross sections and self-consistent flux discontinuity factors, yield results that are in good agreement with fine-mesh nodal *transport* calculations done using lattice-cell size nodes. For the first model, a "small" PWR model which has been studied previously,² the coarse-mesh nodal diffusion calculations based on the systematic homogenization theory yielded an error of -0.078% in

k_{eff} and a maximum error in bundle power of 2.73%, in comparison with the transport values. Analogous coarse-mesh nodal diffusion calculations based on flux and volume weighted (FVW) homogenized diffusion coefficients and cross sections resulted in errors of -0.310% and 5.71% for these quantities when no flux discontinuity factors were used, and -0.086% and 3.09% when the discontinuity factors were used in conjunction with the FVW parameters which is the procedure that results from generalized equivalence theory³(GET). For the second model, a considerably more difficult "large" PWR model described below, the SHT-based coarse-mesh nodal diffusion calculation yielded - 0.143% error in k_{eff} and -4.93% maximum error in bundle power, whereas the FVW-based calculation gave -0.623% and -6.24% for these quantities and the GET-based calculation (FVW plus discontinuity factors) led to -0.235% and -12.14% errors.

The first model studied has been described previously,⁴ and is comprised of a water reflector and a core made up of 69 bundles of three types -- fresh fuel with water holes, partially burned fuel with water holes, and fresh fuel with control rods. According to the original model the 64 cells (8 x 8) in each bundle already are homogeneous;⁴ hence, only the 69 assemblies -- each treated as a single node in the NGFM^{5,6} global diffusion calculation -- had to be homogenized. This was done using the analytically derived SHT-based expressions with the spatial flux and adjoint distributions needed in these expressions¹ computed using an S_4 discrete nodal transport method (DNTM)^{6,7} calculation on a lattice-cell size mesh with periodic boundary conditions. The resulting bundle-homogenized parameters then were used in the global NGFM coarse-mesh calculation. As reported above, the errors that resulted from this calculation were small when comparison was made with a global (whole system) fine-mesh S_4 DNTM (*transport*) calculation on a lattice-cell size mesh.

Hence, a more difficult large PWR model problem was developed to provide a more stringent test.

The large PWR model represents a system with a reflector and a core comprised of 193 fuel assemblies of five types -- fresh fuel (E1), fresh fuel with control rods (C1), partially burned fuel (E2), partially burned fuel with control rods (C2), and spiked fuel (E3). The Nuclear parameters for this test problem are given in Table 1a, and the geometry is shown in Table 1b. The center of the one-eighth core symmetric reactor is at the center of the lower left assembly in Table 1b. Each of 193 bundles was represented by a single node in the 17 x 17 coarse-mesh NGFM global diffusion computation, with the remaining 96 equal size nodes in the reflector. Each bundle is 22.4 cm x 22.4 cm and contains 16 x 16 homogeneous cells, 20 of which are holes for water or control rods (as shown in the inset in Table 1b). The computed assembly power distributions (and per cent errors) are given in Table 1b in which they are compared with the reference solution generated by a very detailed fine-mesh S_4 DNTM (*transport*) calculation on a lattice-cell size mesh. Also shown are the power distributions and per cent errors that resulted from an analogous 17 x 17 NGFM diffusion calculation based on the GET assembly homogenized parameters and discontinuity factors. Clearly, the systematically homogenized coarse-mesh nodal *diffusion* calculation yields a small error in k_{eff} (-0.143%) and small errors in the assembly powers (-4.93% maximum) when compared with the very fine mesh *transport theory* reference solution. Further, the results based on the SHT are more accurate than those based on the GET assembly homogenization procedures, the k_{eff} error and maximum error in assembly power being factors of 1.65 and 2.46 smaller. The L_1 percentage error in the assembly powers, 2.0536 vs. 4.7955 also is a factor of 2.34 smaller.

Table 1a. Nuclear Parameters for the Large PWR Problem

Nuclear Parameters	Fresh Fuel	Partially Burned Fuel	Spiked Fuel	Control Rod	Water
Σ_T	0.2474	0.2381	0.2290	0.3340	0.5770
Σ_a	0.0209	0.0222	0.0223	0.2000	0.0300
$\nu\Sigma_f$	0.0264	0.0303	0.0303	0.0000	0.0000

Table 1b. Assembly Powers and Per Cent Errors in Coarse-Mesh Nodal Diffusion Calculations.

E3	0.8588	E3	0.8667	E3	0.7163	E3	0.4923	--- Fine-Mesh Nodal Transport --- GET Coarse-Mesh Nodal Diffusion --- GET C-M Nodal Diff. % Error --- SHT Coarse-Mesh Nodal Diffusion --- SHT C-M Nodal Diff. % Error
	0.7551		0.7615		0.6360		0.4435				
	-12.07		-12.14		-11.21		-9.90				
	0.8164		0.8258		0.6865		0.4751				
	-4.93		-4.73		-4.15		-3.48				
C2	0.4718	E2	0.5814	C1	0.4229	E2	0.4399	E3	0.4581	E3	0.2612
	0.4314		0.5409		0.3871		0.4114		0.4269		0.2416
	-8.57		-6.95		-8.47		-6.49		-6.81		-7.51
	0.4498		0.5645		0.4050		0.4307		0.4489		0.2508
	-4.66		-2.89		-4.22		-2.10		-2.02		-3.99
E2	0.5634	C1	0.4725	E2	0.4282	C1	0.2970	E2	0.3128	C2	0.2116
	0.5769		0.4704		0.4371		0.2925		0.3058		0.1998
	2.39		-0.46		2.08		-1.53		-2.23		-5.57
	0.5643		0.4622		0.4285		0.2913		0.3095		0.2052
	0.15		-2.19		0.07		-1.93		-1.04		-2.99
C1	1.0341	E2	1.1844	C1	0.6617	E2	0.4215	C1	0.2537	E2	0.3128
	1.0560		1.2248		0.6791		0.4469		0.2539		0.3058
	2.12		3.41		2.63		6.03		0.08		-2.23
	1.0375		1.1984		0.6617		0.4290		0.2464		0.3095
	0.33		1.18		0.00		1.79		-2.86		-1.04
E2	2.2507	E1	2.3739	E2	1.3998	C1	0.6231	E2	0.4215	C1	0.2970
	2.3107		2.4256		1.4525		0.6413		0.4469		0.2925
	2.67		2.18		3.77		2.91		6.03		-1.53
	2.2791		2.4058		1.4190		0.6183		0.4290		0.2913
	1.26		1.34		1.37		-0.77		1.79		-1.93
C1	2.4244	E2	2.9022	C1	1.7474	E2	1.3998	C1	0.6617	E2	0.4282
	2.4586		2.9743		1.7814		1.4525		0.6791		0.4371
	1.41		2.48		1.94		3.77		2.63		2.08
	2.4379		2.9412		1.7578		1.4190		0.6617		0.4285
	0.56		1.34		0.60		1.37		0.00		0.07
E2	3.7163	E1	4.0380	E2	2.9022	E1	2.3739	E2	1.1844	C1	0.4725
	3.7985		4.0973		2.9743		2.4256		1.2248		0.4704
	2.21		1.47		2.48		2.18		3.41		-0.46
	3.7656		4.0861		2.9412		2.4058		1.1984		0.4622
	1.32		1.19		1.34		1.34		1.18		-2.19
C1	3.0600	E2	3.7163	C1	2.4244	E2	2.2507	C1	1.0341	E2	0.5634
	3.0950		3.7985		2.4586		2.3107		1.0560		0.5769
	1.14		2.21		1.41		2.67		2.12		2.39
	3.0754		3.7656		2.4379		2.2791		1.0375		0.5643
	0.51		1.32		0.56		1.26		0.33		0.15
E3	0.8588	E3	0.8667	E3	0.7163	E3	0.4923	E3	0.4581	E3	0.2612
	0.7551		0.7615		0.6360		0.4435		0.4269		0.2416
	-12.07		-12.14		-11.21		-9.90		-6.81		-7.51
	0.8164		0.8258		0.6865		0.4751		0.4489		0.2508
	-4.93		-4.73		-4.15		-3.48		-2.02		-3.99

E1 -- Fresh fuel pins and water holes (SHT Data: $D=1.231627473$, $\Sigma_a=0.02164000225$, $\nu\Sigma_f=0.0244428200$).
 E2 -- Partially burned fuel pins and water holes ($D=1.272761557$, $\Sigma_a=0.02284344485$, $\nu\Sigma_f=0.02398053630$).
 E3 -- Spiked fuel pins and water holes ($D=1.315796654$, $\Sigma_a=0.02293578505$, $\nu\Sigma_f=0.02805356223$).
 C1 -- Fresh fuel pins and control rods ($D=1.306382750$, $\Sigma_a=0.03333460418$, $\nu\Sigma_f=0.02494257448$).
 C2 -- Partially burned fuel pins and control rods ($D=1.352515449$, $\Sigma_a=0.03457567036$, $\nu\Sigma_f=0.02446589739$).

PART III: MULTIPLE-SCALES HOMOGENIZATION OF THE DIFFUSION EQUATION FOR COARSE-MESH CALCULATIONS

INTRODUCTION TO PART III

Modern coarse-mesh nodal methods have proven to be capable of determining fuel-assembly-averaged power distributions with high accuracy and high efficiency, even when the calculations are done on assembly-size grids¹. Thus, it has been recognized for some time that, if the full benefit of these nodal methods are to be realized, accurate assembly homogenization techniques must be developed to provide the homogenized nuclear data for use in the assembly-size-mesh calculations. Toward this end Koebeke² developed equivalence theory (ET)² in which heterogeneity factors, ratios of computed global diffusion theory fluxes to assumed exact or reference fluxes, are introduced in order to reproduce the reference node averaged fluxes and reaction rates and the node-surface averaged partial currents in the coarse-mesh calculations. Smith³ modified this equivalence theory to obtain generalized equivalence theory (GET) in which flux and volume weighted homogenized parameters are used and flux discontinuity factors are introduced. These homogenization theories represent important progress and in fact yield rather accurate results when incorporated into coarse-mesh nodal calculations. However, they are developed in a somewhat ad hoc manner and appear not to have systematic mathematical bases.

In order to develop a self-consistent and systematic lattice-cell and fuel-bundle homogenization theory, we carried out the multiple-scales asymptotic analysis, starting from the transport equation and using three spatial scales,^{4,5} that was summarized in Part I of this report. The numerical results from coarse-mesh nodal diffusion calculations based on the

resulting systematic homogenization theory applied to large 2-D PWR models, which were summarized in Part II, were in good agreement with the results of fine-mesh fully-heterogeneous nodal transport calculations. However, since many analyses of practical thermal reactor problems begin from diffusion theory descriptions, we also have developed a systematic homogenization theory for such calculations. The development, which starts from the diffusion equation and is based on a multiple-scales asymptotic analysis, leads to self-consistent assembly homogenized parameters and flux discontinuity factors. A related earlier development has been reported⁶, however an error was made in that work which led to the omission of certain cross derivatives between different spatial scales, greatly simplified the analysis, and resulted in the omission of terms in the elements of the diffusion tensor. In the present development, we introduce two spatial scales -- a fast or assembly scale and a slow or reactor scale -- and use asymptotic expansions in a small parameter ϵ , the ratio of the mean free path to the characteristic reactor dimension. The development systematically leads to an assembly-homogenized global diffusion equation with explicit self-consistent expressions for the diffusion coefficient (tensor) and the cross sections, and self-consistent flux discontinuity factors.

DEVELOPMENT OF THE SYSTEMATIC HOMOGENIZATION THEORY

The development of the systematic homogenization theory begins from the one-group neutron diffusion equation for a large 3-D heterogeneous system composed of a near-periodic 2-D array of fuel assemblies

$$-\nabla_{\vec{r}} \cdot \mathcal{D}(\vec{r}) \nabla_{\vec{r}} \phi(\vec{r}) + \Sigma_a(\vec{r}) \phi(\vec{r}) = \frac{1}{k_{eff}} \nu \Sigma_f(\vec{r}) \phi(\vec{r}) \quad (1)$$

into which two spatial scales

$$\xi_i = \frac{x_i}{\lambda}, \quad i=1,2; \quad \vec{\zeta} = \epsilon \frac{\vec{r}}{R}$$

are introduced to form the diffusion equation in dimensionless variables

$$\begin{aligned} & -\left(\frac{\partial}{\partial \xi_1} \mathcal{D}^{\zeta}(\xi_1, \xi_2) \frac{\partial}{\partial \xi_1} + \frac{\partial}{\partial \xi_2} \mathcal{D}^{\zeta}(\xi_1, \xi_2) \frac{\partial}{\partial \xi_2}\right) \phi(\xi_1, \xi_2, \vec{\zeta}) \\ & -\epsilon \left(\frac{\partial}{\partial \xi_1} \mathcal{D}^{\zeta}(\xi_1, \xi_2) \frac{\partial}{\partial \zeta_1} + \frac{\partial}{\partial \zeta_1} \mathcal{D}^{\zeta}(\xi_1, \xi_2) \frac{\partial}{\partial \xi_1}\right) \phi(\xi_1, \xi_2, \vec{\zeta}) \\ & -\epsilon \left(\frac{\partial}{\partial \xi_2} \mathcal{D}^{\zeta}(\xi_1, \xi_2) \frac{\partial}{\partial \zeta_2} + \frac{\partial}{\partial \zeta_2} \mathcal{D}^{\zeta}(\xi_1, \xi_2) \frac{\partial}{\partial \xi_2}\right) \phi(\xi_1, \xi_2, \vec{\zeta}) \\ & -\epsilon^2 \nabla_{\vec{\zeta}} \cdot \mathcal{D}^{\zeta} \nabla_{\vec{\zeta}} \phi(\xi_1, \xi_2, \vec{\zeta}) + \sigma_a^{\zeta}(\xi_1, \xi_2) \phi(\xi_1, \xi_2, \vec{\zeta}) = \frac{1}{k_{eff}} \nu \sigma_f^{\zeta}(\xi_1, \xi_2) \phi(\xi_1, \xi_2, \vec{\zeta}) \end{aligned} \quad (2)$$

where ξ_1 is the fast scale which accounts for the spatial variation of the flux within the assembly and $\vec{\zeta}$ is the slow scale which describes the variation of the flux across the overall reactor core. The small parameter ϵ is the ratio of the mean free path to the characteristic reactor dimension.

We expand ϕ and $1/k_{eff}$ in powers of ϵ , substitute the expansions into Eq.(2), and set the coefficients of the various powers of ϵ equal to zero. The ϵ^0 order equation is

$$\begin{aligned}
F\phi_0 = & - \left(\frac{\partial}{\partial \xi_1} D^{\zeta}(\xi_1, \xi_2) \frac{\partial}{\partial \xi_1} + \frac{\partial}{\partial \xi_2} D^{\zeta}(\xi_1, \xi_2) \frac{\partial}{\partial \xi_2} \right) \phi_0(\xi_1, \xi_2, \vec{\zeta}) \\
& + \sigma_a^{\zeta}(\xi_1, \xi_2) \phi_0(\xi_1, \xi_2, \vec{\zeta}) - \frac{1}{k_0} \nu \sigma_f^{\zeta}(\xi_1, \xi_2) \phi_0(\xi_1, \xi_2, \vec{\zeta}) = 0
\end{aligned} \tag{3}$$

where the coefficients depend parametrically on $\vec{\zeta}$. The solution is

$$\phi_0(\xi_1, \xi_2, \vec{\zeta}) = A_0(\vec{\zeta}) \phi^{(0), \vec{\zeta}}(\xi_1, \xi_2) \tag{4}$$

where $\phi^{(0), \vec{\zeta}}$ is the assembly fundamental eigenfunction corresponding to the fundamental eigenvalue $1/k_0^{\vec{\zeta}}$, both of which depend parametrically on the slow variable $\vec{\zeta}$. The coefficient $A_0(\vec{\zeta})$ is a yet to be determined function.

The ϵ^1 order equation is

$$\begin{aligned}
F\phi_1 = & \left(\frac{\partial}{\partial \xi_1} D^{\zeta}(\xi_1, \xi_2) \frac{\partial}{\partial \zeta_1} + \frac{\partial}{\partial \zeta_1} D^{\zeta}(\xi_1, \xi_2) \frac{\partial}{\partial \xi_1} \right) \phi_0 \\
& + \left(\frac{\partial}{\partial \xi_2} D^{\zeta}(\xi_1, \xi_2) \frac{\partial}{\partial \zeta_2} + \frac{\partial}{\partial \zeta_2} D^{\zeta}(\xi_1, \xi_2) \frac{\partial}{\partial \xi_2} \right) \phi_0 + \frac{1}{k_1} \nu \sigma_f^{\zeta}(\xi_1, \xi_2) \phi_0
\end{aligned} \tag{5}$$

Applying the Fredholm alternative theorem gives the solvability condition

$$\begin{aligned}
\langle \phi^{(0), \vec{\zeta} \dagger}, \left(\frac{\partial}{\partial \xi_1} D^{\zeta} \frac{\partial}{\partial \zeta_1} + \frac{\partial}{\partial \zeta_1} D^{\zeta} \frac{\partial}{\partial \xi_1} \right) \phi_0 \rangle + \langle \phi^{(0), \vec{\zeta} \dagger}, \left(\frac{\partial}{\partial \xi_2} D^{\zeta} \frac{\partial}{\partial \zeta_2} + \frac{\partial}{\partial \zeta_2} D^{\zeta} \frac{\partial}{\partial \xi_2} \right) \phi_0 \rangle \\
+ \frac{1}{k_1} \langle \phi^{(0), \vec{\zeta} \dagger}, \nu \sigma_f^{\zeta} \phi_0 \rangle = 0
\end{aligned} \tag{6}$$

or

$$\begin{aligned}
& \frac{1}{k_1} \langle \phi^{(0),\zeta^\dagger}, \nu \sigma_f^\zeta \phi^{(0)} \rangle_{A_0} + \Gamma_1 \frac{\partial A_0}{\partial \zeta_1} + \Gamma_2 \frac{\partial A_0}{\partial \zeta_2} \\
& + \langle \phi^{(0),\zeta^\dagger}, \frac{\partial}{\partial \xi_1} \phi^{(0),\zeta} \frac{\partial D^\zeta}{\partial \zeta_1} + D^\zeta \frac{\partial^2}{\partial \xi_1 \partial \zeta_1} \phi^{(0),\zeta} \rangle_{A_0} \\
& + \langle \phi^{(0),\zeta^\dagger}, \frac{\partial}{\partial \xi_2} \phi^{(0),\zeta} \frac{\partial D^\zeta}{\partial \zeta_2} + D^\zeta \frac{\partial^2}{\partial \xi_2 \partial \zeta_2} \phi^{(0),\zeta} \rangle_{A_0} = 0
\end{aligned} \tag{7}$$

where $\phi^{(0),\zeta^\dagger}$ is the assembly fundamental adjoint eigenfunction. For symmetric assemblies of interest in PWRs, especially at the beginning of life,

$$\begin{aligned}
\Gamma_1 & \equiv \langle \phi^{(0),\zeta^\dagger}, (\frac{\partial}{\partial \xi_1} D^\zeta + D^\zeta \frac{\partial}{\partial \xi_1}) \phi^{(0),\zeta} \rangle = 0 \\
\Gamma_2 & \equiv \langle \phi^{(0),\zeta^\dagger}, (\frac{\partial}{\partial \xi_2} D^\zeta + D^\zeta \frac{\partial}{\partial \xi_2}) \phi^{(0),\zeta} \rangle = 0
\end{aligned} \tag{8}$$

Therefore

$$\begin{aligned}
\frac{1}{k_1^\zeta} & = -\frac{1}{\langle \phi^{(0),\zeta^\dagger}, \nu \sigma_f^\zeta \phi^{(0),\zeta} \rangle} \left[\langle \phi^{(0),\zeta^\dagger}, \frac{\partial}{\partial \xi_1} \phi^{(0),\zeta} \frac{\partial D^\zeta}{\partial \zeta_1} + D^\zeta \frac{\partial^2}{\partial \xi_1 \partial \zeta_1} \phi^{(0),\zeta} \rangle \right. \\
& \quad \left. + \langle \phi^{(0),\zeta^\dagger}, \frac{\partial}{\partial \xi_2} \phi^{(0),\zeta} \frac{\partial D^\zeta}{\partial \zeta_2} + D^\zeta \frac{\partial^2}{\partial \xi_2 \partial \zeta_2} \phi^{(0),\zeta} \rangle \right]
\end{aligned} \tag{9}$$

where the parametric dependence upon $\vec{\zeta}$ has now been indicated in $1/k_1^\zeta$.

The solution for ϕ_1 is

$$\phi_1 = f^\zeta(\xi_1, \xi_2) \frac{\partial A_0}{\partial \zeta_1} + g^\zeta(\xi_1, \xi_2) \frac{\partial A_0}{\partial \zeta_2} + q^\zeta(\xi_1, \xi_2) A_0 \tag{10}$$

where f^ζ , g^ζ , and q^ζ are the particular solutions to the equations

$$Ff^\zeta = \frac{\partial}{\partial \xi_1} D^\zeta \phi^{(0),\zeta} + D^\zeta \frac{\partial}{\partial \xi_1} \phi^{(0),\zeta} \tag{11a}$$

$$Fg^{\zeta} = \frac{\partial}{\partial \xi_2} D^{\zeta} \phi^{(0),\zeta} + D^{\zeta} \frac{\partial}{\partial \xi_2} \phi^{(0),\zeta} \quad (11b)$$

$$Fq^{\zeta} = \frac{1}{k_1^{\zeta}} v \sigma_f^{\zeta} \phi^{(0),\zeta} \quad (11c)$$

Finally, the ϵ^2 order equation is

$$\begin{aligned} F\phi_2 = & \nabla_{\zeta} \cdot D^{\zeta} \nabla_{\zeta} \phi_0 + \left(\frac{\partial}{\partial \xi_1} D^{\zeta} \frac{\partial}{\partial \zeta_1} + \frac{\partial}{\partial \zeta_1} D^{\zeta} \frac{\partial}{\partial \xi_1} \right) \phi_1 \\ & + \left(\frac{\partial}{\partial \xi_2} D^{\zeta} \frac{\partial}{\partial \zeta_2} + \frac{\partial}{\partial \zeta_2} D^{\zeta} \frac{\partial}{\partial \xi_2} \right) \phi_1 + \frac{1}{k_1^{\zeta}} v \sigma_f^{\zeta} \phi_1 + \frac{1}{k_2} v \sigma_f^{\zeta} \phi_0 \end{aligned} \quad (12)$$

Applying the Fredholm alternative theorem again, truncating the expansion of $1/k_{eff}$ at order ϵ^2 , and transforming back to dimensional variables, we obtain the assembly homogenized diffusion equation

$$\nabla_{\zeta} \cdot \underline{D}' \nabla_{\zeta} A_0(\vec{r}) + \left(\frac{1}{k_{eff}} \overline{v \Sigma_f'} - \overline{\Sigma_a'} \right) A_0(\vec{r}) + \underline{V}' \cdot \nabla_{\zeta} A_0(\vec{r}) + S' A_0(\vec{r}) = 0 \quad (13)$$

The explicit expressions for the elements of the homogenized diffusion tensor and the homogenized cross sections are included in the appendix. The expressions for $\underline{V}'$ and S' -- the coefficients for the drift term and the source term, both of which arise in most homogenization theories based on asymptotic expansions -- also are given in the appendix. From the developments above, it follows that the asymptotic solution to the heterogeneous reactor diffusion equation is obtained to the leading order as

$$\phi(\vec{r}) = A_0(\vec{r})\phi^{(0),f}(\vec{r}) + O(\epsilon)$$

where $\phi^{(0),f}(\vec{r})$, the solution to Eq. (3), is the rapidly varying unit heterogeneous assembly eigenfunction and $A_0(\vec{r})$, the solution to Eq. (13), is the slowing varying homogenized global diffusion equation eigenfunction.

The continuity of the heterogeneous (true) flux at assembly interfaces

$$A_0^+ \phi^{(0),f+} = A_0^- \phi^{(0),f-} \quad (14)$$

gives the discontinuity conditions at the interfaces

$$\frac{A_0^+}{A_0^-} = \frac{\phi^{(0),f-}}{\phi^{(0),f+}} \quad (15)$$

that are to be used in obtaining the solution (e.g., via a coarse-mesh nodal method) to Eq. (13), the homogenized global diffusion equation. The value of k_{eff} calculated from this homogenized equation has a third order error in the small parameter ϵ in comparison with that calculated from the original heterogeneous diffusion equation.

TEST PROBLEMS

Three test problems have been studied. The first, a one-dimensional problem, is a slab reactor model comprised of 12 assemblies, 6 on each side of a plane of symmetry. They are of two types -- one with two fuel regions (9 cm each) and a water channel (2 cm) in the center (type W), and the other with two fuel regions (9 cm each) and a control rod channel (2 cm) in the center (type R). The assembly pitch is 20 cm. The nuclear data is given in Table

1a. The assembly homogenization based on the systematically derived expressions was done using the forward and adjoint fluxes calculated using the nodal Green's function method (NGFM)⁷ to solve the assembly diffusion equation with periodic boundary conditions, i.e. to solve Eq. (3). The resulting assembly-homogenized parameters then were used in the global NGFM coarse-mesh calculation. The results of the coarse-mesh calculation are compared with a fine-mesh (9 nodes per assembly) global heterogeneous NGFM calculation in Table 1b in which the powers and per cent errors are tabulated for the 6 assemblies to the right of the symmetry plane. As shown in the table, the calculation based on the systematic homogenization theory (SHT) yielded a -0.31% error in k_{eff} and a maximum error in assembly power of 7.23% in comparison with the fine-mesh heterogeneous calculation. An analogous coarse-mesh NGFM calculation based on GET³ resulted in errors of -0.45% and 14.22% for these quantities.

Table 1a: Nuclear Parameters for the Slab Reactor Model.

Nuclear Parameter	Fuel	Water	Control Rod
D	1.0	0.09998	0.10498
Σ_a	0.022	0.0222	0.0422
$\nu\Sigma_f$	0.027	0.0	0.0

Table 1b: Assembly Powers and Per Cent Error in Coarse-Mesh
NGFM Calculations

1.6620	1.2900	1.2906	1.0599	0.5343	0.1632	--Fine Mesh NGFM
1.6299	1.3284	1.2843	1.0207	0.5502	0.1864	--GET C-M NGFM
-1.93	2.98	-0.49	-3.70	2.98	14.22	--GET C-M% Error
1.6427	1.3146	1.2853	1.0378	0.5445	0.1750	--SHT C-M NGFM
-1.16	1.91	-0.41	-2.09	1.91	7.23	--SHT C-M% Error
W	R	W	W	R	W	--Type of Assembly

W -- Fuel and Water Channel ($D = 0.8098764132$, $\Sigma_a = 0.02226038359$,
 $\nu\Sigma_f = 0.02487388153$).

R -- Fuel and Control Rod Channel ($D = 0.7320592870$, $\Sigma_a = 0.02403712847$,
 $\nu\Sigma_f = 0.02523135245$).

k_{eff} -- Fine Mesh: 1.0930673; GET C-M: 1.0882063(-0.45%);
SHT C-M: 1.0897028(-0.31%).

The second test problem is a small 2-D PWR model. It is composed of a water reflector and a core made up of 69 bundles of three types -- fresh fuel with water holes; partially burned fuel with water holes, and fresh fuel with control rods. The core has quarter-core symmetry about the center of the middle assembly, and each assembly is 12 cm x 12 cm and contains 64 (8 x 8) homogeneous cells. The nuclear data is given in Table 2a. The results of the coarse-mesh NGFM calculations based on the systematic homogenization theory, and those based on generalized equivalence theory³, are compared with a fine mesh (64 nodes per assembly) global heterogeneous NGFM calculation in Table 2b. As can be seen from that table, the coarse-mesh nodal diffusion calculations based on the systematic homogenization theory yielded an error of -0.075% in k_{eff} , a maximum error in assembly power of 5.07% and an L_1 error of 2.30% in comparison with the results of the fine-mesh heterogeneous nodal diffusion calculation. The analogous coarse-mesh nodal diffusion calculation

based on GET parameters yielded -0.089% error in k_{eff} , 8.10% maximum assembly power error, and an L_1 error of 2.54%.

Table 2a: Nuclear Parameters for the 2-D Small PWR Model

Nuclear Parameters	Fresh Fuel	Partially Burned Fuel	Water	Control Rod
D	0.29	0.29	0.146	0.146
Σ_a	0.066	0.066	0.022	0.240
$\nu\Sigma_f$	0.070	0.067	0.000	0.000

**Table 2b: Assembly powers and per cent Errors in Coarse-Mesh
NGFM Calculations.**

E2	0.2580 0.2666 3.33 0.2600 0.78	E2	0.1895 0.2060 8.71 0.1991 5.07	E2	0.1174 0.1254 6.81 0.1212 3.24	-- F-M Nodal Diffusion -- GET C-M Nodal Diff. -- GET C-M Nodal Diff.% Error -- SHT C-M Nodal Diff. -- SHT C-M Nodal Diff.% Error
E1	0.7564 0.7910 4.57 0.7777 2.82	C	0.5281 0.5109 -3.26 0.5076 -3.88	E2	0.3419 0.3616 5.76 0.3519 2.93	0.1580 0.1708 E2 8.10 0.1653 4.62
C	1.5657 1.5004 -4.17 1.5085 -3.65	E1	1.8736 1.8971 1.25 1.9034 1.59	C	0.8412 0.8091 -3.82 0.8115 -3.53	0.3419 0.3616 E2 5.76 0.3519 2.93 E2 0.1174 0.1254 6.81 0.1212 3.24
E1	3.4384 3.4677 0.85 3.4826 1.29	E1	3.3501 3.3778 0.83 3.3917 1.24	E1	1.8736 1.8971 1.25 1.9034 1.59	0.5281 0.5109 C -3.26 0.5076 -3.88 E2 0.1895 0.2060 8.71 0.1991 5.07
C	2.7821 2.6586 -4.44 2.6771 -3.77	E1	3.4384 3.4677 0.85 3.4826 1.29	C	1.5657 1.5004 -4.17 1.5085 -3.65	0.7564 0.7910 E1 4.57 0.7777 2.82 E2 0.2580 0.2666 3.33 0.2600 0.78

E1 -- Fresh Fuel Pins and Water Holes (SHT Data: $D = 0.2807607565$,
 $\Sigma_a = 0.06336805849$, $\nu\Sigma_f = 0.06592623215$)

E2 -- Partially Burned Fuel Pins and Water Holes ($D = 0.2807607565$,
 $\Sigma_a = 0.06336805849$, $\nu\Sigma_f = 0.063310082220$)

C -- Fresh Fuel Pins and Control Rods ($D = 0.2713814544$, $\Sigma_a = 0.07354185062$,
 $\nu\Sigma_f = 0.06696592216$)

k_{eff} -- Fine Mesh: 0.99833306; GET C-M: 0.99744997(-0.089);
SHT C-M: 0.99758155(-0.075%).

Finally, the new systematic homogenization theory has been applied to a large PWR model core with 193 assemblies of 5 types -- shown in Table 3. This problem also was solved via coarse-mesh NGFM⁷ calculations on assembly-size meshes, based on both SHT and GET parameters, and the results were compared with the fine mesh NGFM reference solutions generated using lattice-cell size meshes. For this problem, the SHT also led to more accurate results than the GET, but the improvement was less significant. The computed assembly power distribution (and per cent errors) based on both are given in Table 3b. The former resulted in an error of -0.0104% in k_{eff} , a maximum error of 8.52% in assembly power, and an L_1 error of 1.53% when compared with the fine lattice-cell size mesh NGFM reference solution, while the latter led to -0.0109%, 9.25% and 1.73%, respectively.

Table 3a. Nuclear Data for the Large PWR Problem

Nuclear Parameters	Fresh Fuel	Partially Burned Fuel	Spiked Fuel	Control Rod	Water	Reflector
D	0.3900	0.3790	0.3900	0.1360	0.1420	0.8400
Σ_a	0.0676	0.0680	0.0676	0.0500	0.0220	0.0010
$\nu\Sigma_f$	0.0708	0.0704	0.0710	0.0000	0.0000	0.0000

Table 3b. Shown in each assembly are assembly powers and per cent errors in coarse-mesh nodal diffusion calculations. The core has quarter-core symmetry about the center of the middle assembly. Each bundle is 20cm x 20cm and contains 16 x 16 homogeneous cells, 20 of which are holes for water or control rods. Each of the 193 assemblies is represented by a single node in the 17 x 17 coarse-mesh NGFM⁷ global diffusion computation, with the remaining 96 equal size nodes in the reflector.

0.2495 0.2669 E3 6.97 0.2653 6.33	0.2553 0.2718 E3 6.46 0.2702 5.84	0.2274 0.2459 E3 8.14 0.2444 7.48	0.1795 0.1961 E3 9.25 0.1948 8.52	-- Fine-Mesh Nodal Diffusion -- GET Coarse-Mesh Nodal Diffusion -- GET C-M Nodal Diff. % Error -- SIIT Coarse-Mesh Nodal Diffusion -- SIIT C-M Nodal Diff. % Error		Heterogeneous Fuel Assembly with Control-Rod/Water Holes Shown	
0.3568 0.3654 C2 2.41 0.3639 1.99	0.3929 0.4120 E2 4.86 0.4095 4.22	0.3318 0.3457 C1 4.19 0.3442 3.74	0.2975 0.3196 E2 7.43 0.3174 6.69	0.2458 0.2661 E3 8.26 0.2644 7.57	0.1504 0.1632 E3 8.51 0.1620 7.71		
0.7107 0.7257 E2 2.11 0.7230 1.73	0.6428 0.6482 C1 0.84 0.6470 0.65	0.5591 0.5769 E2 3.18 0.5741 2.68	0.3996 0.4135 C1 3.48 0.4118 3.05	0.3142 0.3347 E3 6.52 0.3323 5.76	0.1955 0.2077 C2 6.24 0.2064 5.58	0.1504 0.1632 E3 8.51 0.1620 7.71	K_{eff} -- 1.0044434 -- 1.0043336 -- -0.0109 -- 1.0043392 -- -0.0104
1.3455 1.3353 C1 -0.76 1.3368 -0.65	1.3832 1.3824 E2 -0.06 1.3817 -0.11	0.9561 0.9558 C1 -0.03 0.9556 -0.05	0.6582 0.6770 E2 2.86 0.6740 2.40	0.4137 0.4247 C1 2.66 0.4229 2.22	0.3142 0.3347 E2 6.52 0.3323 5.76	0.2458 0.2661 E3 8.26 0.2644 7.57	
2.3894 2.3682 E2 -0.89 2.3698 -0.82	2.4279 2.4149 E1 -0.54 2.4170 -0.45	1.6650 1.6615 E2 -0.21 1.6608 -0.25	0.9808 0.9784 C1 -0.24 0.9778 -0.31	0.6582 0.6770 E2 2.86 0.6740 2.40	0.3996 0.4135 C1 3.48 0.4118 3.05	0.2975 0.3196 E2 7.43 0.3174 6.69	0.1795 0.1961 E3 9.25 0.1948 8.52
2.4244 2.4586 C1 -1.84 2.7722 -1.57	2.9755 2.9398 E2 -1.20 2.9433 -1.08	2.1500 2.1182 C1 -1.48 2.1229 -1.26	1.6650 1.6615 E2 -0.21 1.6608 -0.25	0.9561 0.9558 C1 -0.03 0.9556 -0.05	0.5591 0.5769 E2 3.18 0.5741 2.68	0.3318 0.3457 C1 4.19 0.3442 3.74	0.2274 0.2459 E3 8.14 0.2444 7.48
3.6909 3.6367 E2 -1.47 3.6425 -1.31	3.8308 3.7821 E1 -1.27 3.7891 -1.09	2.9755 2.9398 E2 -1.20 2.9433 -1.08	2.4279 2.4149 E1 -0.54 2.4170 -0.45	1.3832 1.3824 E2 -0.06 1.3817 -0.11	0.6428 0.6482 C1 0.84 0.6470 0.65	0.3929 0.4120 E2 4.86 0.4095 4.22	0.2553 0.2718 E3 6.46 0.2702 5.84
3.4541 3.3808 C1 -2.12 3.3915 -1.81	3.6909 3.6367 E2 -1.47 3.6425 -1.31	2.8163 2.7645 C1 -1.84 2.7722 -1.57	2.3894 2.3682 E2 -0.89 2.3698 -0.82	1.3455 1.3353 C1 -0.76 1.3368 -0.65	0.7107 0.7257 E2 2.11 0.7230 1.73	0.3568 0.3654 C2 2.41 0.3639 1.99	0.2495 0.2669 E3 6.97 0.2653 6.33

E1 -- Fresh fuel pins and water holds (SIIT Data: $D=0.3702899838$, $\Sigma_a=0.06425117514$, $\nu\Sigma_f=0.06553233198$)
E2 -- Partially burned fuel pins and water holes ($D=0.3601499485$, $\Sigma_a=0.06462515076$, $\nu\Sigma_f=0.06516665272$)
E3 -- Spiked fuel pins and water holes ($D=0.3702899838$, $\Sigma_a=0.06425117514$, $\nu\Sigma_f=0.06571745157$)
C1 -- Fresh fuel pins and control rods ($D=0.3690446124$, $\Sigma_a=0.06658848866$, $\nu\Sigma_f=0.06585366185$)
C2 -- Partially burned fuel pins and control rods ($D=0.3588950483$, $\Sigma_a=0.06696656956$, $\nu\Sigma_f=0.06549129018$)

SUMMARY OF PART III

Starting from the diffusion equation, a systematic homogenization theory has been developed using a multiple-scales asymptotic expansion which leads to an assembly-homogenized global diffusion equation with explicit self-consistent expressions for the diffusion coefficient (tensor), the cross sections, and the flux discontinuity factors. Application to a simple 1-D test problem and to two 2-D PWR problems showed that the homogenized parameters obtained via the SHT make possible very accurate solutions while using coarse-mesh methods even on assembly size meshes. It also led to more accurate results on those meshes than the GET for both PWR problems.

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Appendix III-A

The explicit expressions for the elements of the homogenized diffusion tensor, the homogenized cross sections, and the coefficients of the drift and source terms, derived in the systematic homogenization theory and used in the global coarse-mesh nodal diffusion calculations are given below. They appear as coefficients in the global diffusion equation, Eq. (13) in Part III.

The elements of the homogenized diffusion tensor are

$$D_{11} = \frac{1}{N} [\langle \phi^{(0),f \dagger}, D^f \phi^{(0),f} \rangle + \langle \phi^{(0),f \dagger}, D^f \frac{\partial}{\partial r_1} f^f + \frac{\partial}{\partial r_1} D^f f^f \rangle]$$

$$D_{12} = \frac{1}{N} \langle \phi^{(0),f \dagger}, (\frac{\partial}{\partial r_1} D^f + D^f \frac{\partial}{\partial r_1}) g^f \rangle$$

$$D_{21} = \frac{1}{N} \langle \phi^{(0),f \dagger}, (\frac{\partial}{\partial r_2} D^f + D^f \frac{\partial}{\partial r_2}) f^f \rangle$$

$$D_{22} = \frac{1}{N} [\langle \phi^{(0),f \dagger}, D^f \phi^{(0),f} \rangle + \langle \phi^{(0),f \dagger}, D^f \frac{\partial}{\partial r_2} g^f + \frac{\partial}{\partial r_2} D^f g^f \rangle]$$

$$D_{33} = \frac{1}{N} \langle \phi^{(0),f \dagger}, D^f \phi^{(0),f} \rangle$$

$$D_{13} = D_{23} = D_{31} = D_{32} = 0 .$$

The homogenized cross sections are

$$\overline{\Sigma_f^f} = \frac{1}{N} \langle \phi^{(0),f \dagger}, \nu \Sigma_f^f \phi^{(0),f} \rangle$$

$$\overline{\Sigma_a^f} = \frac{1}{k_0^f} \overline{\Sigma_f^f} ,$$

and the coefficients of the drift term and source term are

$$\begin{aligned}
V_1^r &= \frac{1}{N} \left[\langle \phi^{(0),r \dagger}, \left(\frac{\partial}{\partial r_1} D^r \frac{\partial}{\partial r_1} - \frac{\partial}{\partial r_1} \left(\frac{\partial}{\partial r_1} D^r \right) \right) f^r \rangle + \frac{1}{k_1^r} \langle \phi^{(0),r \dagger}, v \Sigma_f^r f^r \rangle \right. \\
&\quad - \langle \frac{\partial}{\partial r_1} \phi^{(0),r \dagger}, (D^r \frac{\partial}{\partial r_1} + \frac{\partial}{\partial r_1} D^r) f^r \rangle - \langle \frac{\partial}{\partial r_2} \phi^{(0),r \dagger}, (D^r \frac{\partial}{\partial r_2} + \frac{\partial}{\partial r_2} D^r) f^r \rangle \\
&\quad \left. - \langle \phi^{(0),r \dagger}, \frac{\partial}{\partial r_2} \left(\frac{\partial}{\partial r_2} D^r \right) f^r \rangle + \langle \phi^{(0),r \dagger}, \left(\frac{\partial}{\partial r_1} D^r + D^r \frac{\partial}{\partial r_1} \right) q^r \rangle \right] \\
V_2^r &= \frac{1}{N} \left[\langle \phi^{(0),r \dagger}, \left(\frac{\partial}{\partial r_2} D^r \frac{\partial}{\partial r_2} - \frac{\partial}{\partial r_2} \left(\frac{\partial}{\partial r_2} D^r \right) \right) g^r \rangle + \frac{1}{k_1^r} \langle \phi^{(0),r \dagger}, v \Sigma_f^r g^r \rangle \right. \\
&\quad - \langle \frac{\partial}{\partial r_2} \phi^{(0),r \dagger}, (D^r \frac{\partial}{\partial r_2} + \frac{\partial}{\partial r_2} D^r) g^r \rangle - \langle \frac{\partial}{\partial r_1} \phi^{(0),r \dagger}, (D^r \frac{\partial}{\partial r_1} + \frac{\partial}{\partial r_1} D^r) g^r \rangle \\
&\quad \left. - \langle \phi^{(0),r \dagger}, \frac{\partial}{\partial r_1} \left(\frac{\partial}{\partial r_1} D^r \right) g^r \rangle + \langle \phi^{(0),r \dagger}, \left(\frac{\partial}{\partial r_2} D^r + D^r \frac{\partial}{\partial r_2} \right) q^r \rangle \right] \\
S^r &= \frac{1}{N} \left[\langle \phi^{(0),r \dagger}, \left(\frac{\partial}{\partial r_1} D^r \frac{\partial}{\partial r_1} + \frac{\partial}{\partial r_1} D^r \frac{\partial}{\partial r_1} \right) q^r \rangle + \frac{1}{k_1^r} \langle \phi^{(0),r \dagger}, v \Sigma_f^r q^r \rangle \right. \\
&\quad \left. + \langle \phi^{(0),r \dagger}, \left(\frac{\partial}{\partial r_2} D^r \frac{\partial}{\partial r_2} + \frac{\partial}{\partial r_2} D^r \frac{\partial}{\partial r_2} \right) q^r \rangle - \frac{1}{k_1^r} \langle \phi^{(0),r \dagger}, v \Sigma_f^r \phi^{(0),r} \rangle \right]
\end{aligned}$$

where

$$N = \langle \phi^{(0),r \dagger}, \phi^{(0),r} \rangle.$$

SUMMARY

The main results obtained through the research performed under this grant already have been summarized at the ends of the three major parts of this final report. However, they are re-iterated briefly here for completeness.

The essential result that formed the basis for most of the remainder of the research was the systematic mathematical development of a simultaneous, self-consistent, lattice-cell and fuel-assembly homogenization theory that began from the transport equation, rather than the diffusion equation, and therefore provides both a theoretical basis and practical homogenization procedures for the use of coarse-mesh nodal diffusion methods on fuel-assembly-sized meshes to carry out reactor core calculations that reap the accuracy and efficiency benefits of nodal methods while simultaneously yielding computational results that are comparable to those obtained using fine-mesh nodal *transport* methods. The details of the development of this transport-equation-based systematic homogenization theory were summarized in Part I of this report.

Next, this homogenization theory was validated by solving simple one-dimensional test problems. Those studies also are summarized in Part I above.

Then, rather detailed and extensive applications of this systematic homogenization theory in concert with coarse-mesh nodal diffusion calculations for practical two-dimensional small and large PWR models were carried out. The results of those studies are summarized in Part II of this final report, in which it is shown that the new systematic homogenization theory yields values for k_{eff} and assembly powers that are in better agreement with the fine-mesh nodal transport theory values than are those obtained using

traditional flux and volume weighted homogenization procedures or generalized equivalence theory.

Finally, because some simple analyses of thermal reactors actually begin from the diffusion theory description and not the transport theory description, a separate diffusion-equation-based systematic homogenization theory was developed, validated on simple one-dimensional test problems, and applied to practical two-dimensional small and large PWR core calculations done using coarse-mesh nodal diffusion methods. These results, which are summarized in Part III of this final report, show that this diffusion-equation-based systematic homogenization theory yields results that are in better agreement with the reference solutions, obtained using fine-mesh nodal diffusion methods, than are those obtained using traditional homogenization procedures or the recently developed generalized equivalence theory.

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