Systematic homogenization and self-consistent flux and pin power reconstruction for nodal diffusion methods

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SYSTEMATIC HOMOGENIZATION AND SELF-CONSISTENT FLUX AND PIN POWER RECONSTRUCTION FOR NODAL DIFFUSION METHODS.

PART II: TRANSPORT EQUATION BASED THEORY

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Dedicated to Professor Gerald C. Pomraning
on the Occasion of His Sixtieth Birthday

ABSTRACT

Starting from the transport equation, a systematic homogenization theory and a self-consistent de-homogenization theory for fuel assemblies have been developed using a multiple-scales asymptotic expansion method. The resulting theory provides a framework for coarse-mesh nodal diffusion calculations of light water reactors. The theoretical development is carried out through second order in a small parameter — the ratio of the neutron mean free path to the reactor characteristic dimension. Introducing two spatial scales — a fast scale for the rapid variation of the flux over a fuel assembly and a slow scale for the slow variation of the flux over the whole core — into the neutron transport equation for a three-dimensional heterogeneous medium, the development systematically yields: an assembly-homogenized global diffusion equation with self-consistent expressions for the assembly-homogenized diffusion tensor elements and cross sections, and assembly-surface flux discontinuity factors. The analysis shows that the solution of the assembly-homogenized global diffusion equation leads to a reactor eigenvalue \( \lambda_{\text{eff}} \) that is second order in the small parameter, and

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a heterogeneous transport theory angular flux that is leading order. The resulting framework also provides a natural and self-consistent procedure for the reconstruction of the local heterogeneous angular fluxes which makes it possible to calculate the pin powers.

1 Introduction

In an earlier paper,\(^1\) which will be referred to here as Part I, using a multiple-scales asymptotic expansion method, we developed and applied a diffusion-equation-based systematic fuel assembly homogenization theory (DEB/SHT) and a self-consistent local flux reconstruction procedure. That development, which started from the diffusion equation, exploited the two spatial scales that naturally exist in commercial pressurized water reactors whose three-dimensional cores are made up of near periodic two-dimensional arrays of heterogeneous fuel assemblies comprised of fuel lattice cells. In the design and operation analysis of more advanced thermal reactors, such as those using fuel assemblies with heavy loadings of gadolinium, the transport equation is necessary to perform accurate fuel assembly calculations; hence a development analogous to that in Part I, but starting now from the transport equation rather than the diffusion equation is given here to provide a transport-equation-based systematic homogenization theory (TEB/SHT) for fuel assemblies. As in the DEB/SHT, although unnecessary, the fuel lattice cells are taken as already homogenized, and fast and slow spatial scales, for the assembly and overall core flux variations respectively, are introduced into the transport equation. The angular flux and the reactor eigenvalue then are expanded in a small parameter \(\varepsilon\), which is the ratio of the neutron total mean free path to
the characteristic reactor dimension. Substituting these expansions into the three-dimensional transport equation, collecting the terms with like powers of \( \varepsilon \) and setting them equal to zero, yields a hierarchy of equations. Solving these equations successively leads systematically to an assembly-homogenized reactor diffusion equation with explicit self-consistent expressions for the diffusion tensor, cross-sections, and flux discontinuity conditions at the homogenized assembly interfaces. It also simultaneously leads to a self-consistent de-homogenization procedure for the reconstruction of the local heterogeneous transport theory fluxes. The transport-equation-based systematic homogenization theory that results provides a self-consistent framework within which it is possible to start from homogenized fuel lattice cell nuclear data and carry out coarse-mesh nodal diffusion calculations on assembly-size meshes, to obtain eigenvalues, assembly powers, reconstructed local fluxes, and pin powers of accuracy comparable to those obtained via fine mesh transport calculations using cell size, or finer, meshes.

2 Theoretical Development

The theoretical development of the transport-equation-based systematic homogenization theory for fuel assemblies begins from the eigenvalue problem associated with the one-group neutron transport equation for a large three-dimensional heterogeneous system comprised of a two-dimensional array of near-periodic fuel assemblies

\[
\hat{\Omega} \cdot \nabla \rho \Psi(\vec{r}, \hat{\Omega}) + \Sigma_T(\vec{r}) \Psi(\vec{r}, \hat{\Omega}) = \int_{4\pi} \Sigma_s(\vec{r}, \hat{\Omega} \cdot \hat{\Omega}') \Psi(\vec{r}, \hat{\Omega}') d^2\Omega'
+ \frac{1}{\kappa_{eff}} \nu \Sigma_f(\vec{r}) \int_{4\pi} \Psi(\vec{r}, \hat{\Omega}') d^2\Omega' ,
\]

(1)
where $\Psi(\vec{r}, \vec{\Omega})$ is the angular flux, $\Sigma_j, j = T, s, f$, are the total, scattering and fission cross sections respectively, $\nu$ is the average number of neutrons produced per fission, and $\frac{1}{\kappa_{eff}}$ is the reactor eigenvalue. Two scaled spatial variables are introduced

$$\xi_i = \frac{r_i}{\lambda}, \quad i = 1, 2,$$

and

$$\zeta = \frac{\vec{r}}{\lambda},$$

where the small parameter $\epsilon \equiv \lambda / R$ is the ratio of the reactor-averaged total mean free path $\lambda$ to the reactor characteristic dimension $R$. The fast-scale variable $\xi_i, i = 1, 2,$ is associated with the rapid variation of the flux within the fuel assemblies, while the slow-scale variable $\zeta$ is associated with the slow variation of the overall flux across the reactor core. These scales are analogous to those used by Larsen in the development of a homogenization theory for exactly periodic fuel cell lattices.\(^2,3\) Here, the two spatial scales — which are formally treated as independent — are introduced into Eq. (1) to obtain the dimensionless transport equation

\[
\sqrt{1 - \mu^2 (\cos \phi \frac{\partial}{\partial \xi_1} + \sin \phi \frac{\partial}{\partial \xi_2})} \psi(\xi_1, \xi_2, \zeta, \vec{\Omega}) + \epsilon \vec{\Omega} \cdot \nabla \psi
\]

\[
+ \sigma^T(\xi_1, \xi_2) \psi = \int_{\Omega_{f}} \sigma^f(\xi_1, \xi_2, \hat{\Omega} \cdot \hat{\Omega'}) \psi d^2 \Omega' + \frac{1}{\kappa_{eff}} \nu \sigma^f(\xi_1, \xi_2) \int_{\Omega_{c}} \psi d^2 \Omega' \quad (2)
\]

where the dimensionless angular flux and cross sections are

$$\psi(\xi_1, \xi_2, \zeta, \vec{\Omega}) = \Psi(\vec{r}, \vec{\Omega})$$

$$\sigma^T_\xi(\xi_1, \xi_2) = \lambda \Sigma_i(\vec{r}) \quad , \quad i = s, T, f.$$
and the trivial scaling of the flux by $\lambda^2 \tau$, where $\tau$ is a characteristic time, has been suppressed. The parametric dependence upon the slow-scale variable $\tilde{\zeta}$, which represents the variation in cross sections from one fuel assembly to another due to fact that the fuel assemblies are only near-periodic, is indicated by the superscripts on the dimensionless cross sections. The angular flux $\psi$ and the eigenvalue $1/k_{ef}$ are expanded in powers of $\epsilon$

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

$$\frac{1}{k_{ef}} = \sum_{n=0}^{\infty} \epsilon^n \frac{1}{\lambda_n} .$$

These expansions are substituted into Eq. (2), and then setting the coefficients of the various powers of $\epsilon$ equal to zero leads to a set of hierarchy equations. The $\epsilon^0$ order equation is

$$F^\tilde{\zeta}\psi_0(\xi_1, \xi_2, \tilde{\zeta}, \hat{\Omega}) \equiv \sqrt{1 - \mu^2} (\cos\phi \frac{\partial}{\partial \xi_1} + \sin\phi \frac{\partial}{\partial \xi_2}) \psi_0 + \sigma^\tilde{\zeta}_2(\xi_1, \xi_2) \psi_0$$

$$- f_0 \sigma^\tilde{\zeta}_2(\xi_1, \xi_2, \tilde{\zeta}, \hat{\Omega}) \psi_0 d^2\Omega' - \frac{1}{\lambda_n} \nu \sigma^\tilde{\zeta}_2(\xi_1, \xi_2) f_0 \psi_0 d^2\Omega' = 0 .$$

This is a transport equation for a family of infinite-medium reactors, each composed of exactly periodic fuel assemblies with cross sections corresponding to a specific value of the slow-scale variable $\tilde{\zeta}$. The general solution to Eq. (5), which also is the transport equation for a unit heterogeneous assembly with periodic boundary conditions, is

$$\psi_0(\xi_1, \xi_2, \tilde{\zeta}, \hat{\Omega}) = A(\tilde{\zeta}) \psi^{(0)}(\xi_1, \xi_2, \tilde{\zeta}, \hat{\Omega}) ,$$

where $\psi^{(0)}(\tilde{\zeta}, \hat{\Omega})$ is the fundamental eigenfunction of the unit fuel assembly transport equation

$$F^\tilde{\zeta}\psi^{(0)}(\xi_1, \xi_2, \tilde{\zeta}, \hat{\Omega}) = 0 ,$$
with periodic boundary conditions (i.e. the fundamental "assembly eigenfunction")
corresponding to the fundamental assembly eigenvalue \(1/k^2_{0,0}\), both of which depend
parametrically upon the slow-scale variable \(\tilde{\zeta}\). \(A_0(\tilde{\zeta})\) is an unknown function which
will be determined from the solution to the higher order equations. The "fuel assembly
fundamental adjoint eigenfunction" satisfies the fuel assembly adjoint transport
equation

\[
F^\dagger \psi^{(0)} \cdot \tilde{\zeta}(\xi_1, \xi_2, \tilde{\Omega}) \equiv -\sqrt{1 - \mu^2} \left( \cos \phi \frac{\partial}{\partial \xi_1} + \sin \phi \frac{\partial}{\partial \xi_2} \right) \psi^{(0)} \cdot \tilde{\zeta} + \sigma F^\dagger(\xi_1, \xi_2) \psi^{(0)} \cdot \tilde{\zeta} \\
- \int_{\Omega} \sigma^F(\xi_1, \xi_2, \tilde{\Omega} \cdot \tilde{\Omega}') \psi^{(0)} \cdot \tilde{\zeta} d\Omega' - \frac{1}{4\pi k_{\text{eff}}} \nu \sigma F(\xi_1, \xi_2) \int_{\Omega} \psi^{(0)} \cdot \tilde{\zeta} d\Omega' = 0 ,
\]

with periodic boundary conditions. Its solution, which will be needed to establish
the solvability conditions for the higher order equations, can be written immediately
in terms of the solution to the assembly (forward) transport equation as

\[
\psi^{(0)} \cdot \tilde{\zeta}(\xi_1, \xi_2, \mu, \phi) = \psi^{(0)} \cdot \tilde{\zeta}(\xi_1, \xi_2, \mu, \phi - \pi) ,
\]
due to the relationship between Eqs. (2) and (5).

The \(\epsilon^1\) order equation is

\[
F^\dagger \psi(\xi_1, \xi_2, \tilde{\zeta}, \Omega) = -\dot{\Omega} \cdot \nabla \psi_0 + \frac{1}{4\pi} \frac{1}{k_1} \nu \sigma F(\xi_1, \xi_2) \int_{\Omega} \psi_0 d\Omega' ,
\]
where the operator \(F^\dagger\) is given by Eq. (5). By the Fredholm alternative theorem,
Eq. (10) has a solution if and only if its right hand side is orthogonal to \(\psi^{(0)} \cdot \tilde{\zeta}\). This
solvability condition yields

\[
- \langle \psi^{(0)} \cdot \tilde{\zeta}, \dot{\Omega} \cdot \nabla (A_0(\tilde{\zeta}) \psi^{(0)} \cdot \tilde{\zeta}) \rangle + \frac{1}{k_1} \psi^{(0)} \cdot \tilde{\zeta} , \nu \sigma F(\xi_1, \xi_2) \psi_0 > = 0 ,
\]
where the inner product $<>$ is the spatial integral over a fuel assembly and the integral over all direction vectors $\hat{\Omega}$, and the scalar flux $\tilde{\psi}_0$ is defined as

$$\tilde{\psi}_0(\xi_0, \xi_1, \zeta) \equiv \frac{1}{4\pi} \int_{4\pi} d^2 \Omega \psi_0(\xi_1, \xi_2, \hat{\Omega}) .$$  \hspace{1cm} (12)$$

Equation (11) now can be solved for $\frac{1}{k_1}$. Writing out the first term on its left hand side as

$$< \psi^{(0)}|^2 (\zeta, \hat{\Omega}) \cdot \nabla \zeta (A_0(\zeta)) > = < \psi^{(0)}|^2 (\zeta, \hat{\Omega}) \cdot \nabla \zeta A_0(\zeta) > + A_0(\zeta) \hat{\Omega} \cdot \nabla \psi^{(0)}(\zeta) ,$$

and noticing that the first term on the right hand side of this expression is identically zero since

$$< \psi^{(0)}|^2 (\zeta, \hat{\Omega}) \cdot \nabla \zeta >= \int_{\text{assembly}} d^2 \xi \int_{0}^{2\pi} d\phi \int_{-1}^{1} d\mu \psi^{(0)}(\zeta)(\xi_1, \xi_2, \mu, \phi - \pi)$$

$$\cdot (1 - \mu^2 (\cos \phi \frac{\partial}{\partial \xi_1} + \sin \phi \frac{\partial}{\partial \xi_2}) + \mu \frac{\partial}{\partial \zeta_3}) A_0(\zeta) = 0 ,$$

it follows that

$$\frac{1}{k_1^2} = \frac{< \psi^{(0)}|^2 (\zeta, \hat{\Omega}) \cdot \nabla \zeta >}{< \psi^{(0)}|^2 (\zeta, \hat{\Omega}) >} ,$$ \hspace{1cm} (13)

where the parametric dependence of $k_1$ upon $\zeta$ has been indicated. The general solution for $\psi_1$ is

$$\psi_1(\xi_1, \xi_2, \zeta, \hat{\Omega}) = A_1(\zeta) \psi^{(0)}(\xi_1, \xi_2, \hat{\Omega}) - f^\zeta(\xi_1, \xi_2, \hat{\Omega}) \frac{\partial A_0}{\partial \zeta}$$

$$- g^\zeta(\xi_1, \xi_2, \hat{\Omega}) \frac{\partial}{\partial \zeta_3} - h^\zeta(\xi_1, \xi_2, \hat{\Omega}) \frac{\partial}{\partial \zeta_3} - [f^\zeta(\xi_1, \xi_2, \hat{\Omega})] A_0$$

$$+ g^\zeta(\xi_1, \xi_2, \hat{\Omega}) + h^\zeta(\xi_1, \xi_2, \hat{\Omega}) - q^\zeta(\xi_1, \xi_2, \hat{\Omega}) ] A_0 ,$$ \hspace{1cm} (15)

where $A_1(\zeta)$ is an unknown function, and $f^\zeta, g^\zeta, h^\zeta, f^\zeta', g^\zeta', h^\zeta'$ and $q^\zeta$ satisfy the
following inhomogeneous assembly transport equations with periodic boundary conditions

\[
F^\xi f^{\xi}(\xi_1, \xi_2, \hat{\Omega}) = \sqrt{1 - \mu^2 \cos \phi \psi^{(0)} \zeta(\xi_1, \xi_2, \hat{\Omega})} \\
F^\xi g^{\xi}(\xi_1, \xi_2, \hat{\Omega}) = \sqrt{1 - \mu^2 \sin \phi \psi^{(0)} \zeta(\xi_1, \xi_2, \hat{\Omega})} \\
F^\xi h^{\xi}(\xi_1, \xi_2, \hat{\Omega}) = \mu \psi^{(0)} \zeta(\xi_1, \xi_2, \hat{\Omega}) \\
F^\xi f^{\xi'}(\xi_1, \xi_2, \hat{\Omega}) = \sqrt{1 - \mu^2 \cos \phi} \frac{\partial \psi^{(0)} \zeta(\xi_1, \xi_2, \hat{\Omega})}{\partial \xi_1} \\
F^\xi g^{\xi'}(\xi_1, \xi_2, \hat{\Omega}) = \sqrt{1 - \mu^2 \sin \phi} \frac{\partial \psi^{(0)} \zeta(\xi_1, \xi_2, \hat{\Omega})}{\partial \xi_2} \\
F^\xi h^{\xi'}(\xi_1, \xi_2, \hat{\Omega}) = \mu \frac{\partial \psi^{(0)} \zeta(\xi_1, \xi_2, \hat{\Omega})}{\partial \xi_3} \\
F^\xi f^{\xi}(\xi_1, \xi_2, \hat{\Omega}) = \frac{1}{k_1^2} \nu \sigma^\xi \bar{\psi}^{(0)}(\xi_1, \xi_2, \hat{\Omega}) .
\]

Applying the Fredholm alternative theorem to the \( \varepsilon^3 \) order equation

\[
F^\xi \psi_2(\xi_1, \xi_2, \bar{\zeta}, \hat{\Omega}) = -\hat{\Omega} \cdot \nabla \psi_1 + \frac{1}{4\pi k_1^2} \nu \sigma^\xi \int_{4\pi} \psi_1 d^2\Omega' + \frac{1}{4\pi k_2^2} \nu \sigma^\xi \frac{1}{\psi_0 d^2\Omega'}
\]

yields the solvability condition

\[
- < \psi^{(0)} \zeta, \hat{\Omega} \cdot \nabla \psi_1 > + < \psi^{(0)} \zeta, \frac{1}{k_1^2} \nu \sigma^\xi \bar{\psi}_1 > + < \psi^{(0)} \zeta, \frac{1}{k_2^2} \nu \sigma^\xi \bar{\psi}_0 > = 0 .
\]

Substituting the expansion of \( \frac{1}{k_{eff}} \) truncated at \( \varepsilon^3 \) order

\[
\frac{1}{k_2^2} = \frac{1}{\varepsilon^3} \left( \frac{1}{k_{eff}} - \frac{1}{k_{0,0}} - \varepsilon \frac{1}{k_1^2} \right) ,
\]

(25)
into Eq. (24), and dividing each term by a normalization factor $N^\xi_i < \psi^{(0)}_0, \psi^{(0)}_i >$, we obtain, after some manipulations, the assembly-homogenized global diffusion equation

$$\nabla^\xi \cdot \overrightarrow{D}^\xi \nabla^\xi A_0(\xi) + \frac{1}{e_i} \left( \frac{1}{k_{\text{eff}}} \overrightarrow{\nu}^\xi \sigma_f^\xi - \overrightarrow{\sigma}^\xi \right) A_0 + \overrightarrow{\Gamma}^\xi \cdot \nabla^\xi A_0 + \overrightarrow{\Phi}^\xi A_0 = 0 \quad (26)$$

where the assembly-homogenized diffusion tensor is

$$\overrightarrow{D}^\xi = \frac{1}{N^\xi_i} \left[ \begin{array}{ccc} < \psi^{(0)}_0 \xi, \sqrt{1 - \mu^2 \cos f^\xi} > & < \psi^{(0)}_0 \xi, \sqrt{1 - \mu^2 \cos \phi^\xi} > & 0 \\ < \psi^{(0)}_0 \xi, \sqrt{1 - \mu^2 \sin f^\xi} > & < \psi^{(0)}_0 \xi, \sqrt{1 - \mu^2 \sin \phi^\xi} > & 0 \\ 0 & 0 & < \psi^{(0)}_0 \xi, \mu_h^\xi > \end{array} \right]$$

The off-diagonal elements of the diffusion tensor become zero, if the fuel assembly is 90°-degree-rotationally symmetric. The assembly-homogenized cross sections are

$$\overrightarrow{\nu}^\xi = \frac{1}{N^\xi_i} < \psi^{(0)}_0 \xi, \nu_{\sigma_f} \sigma_f^\xi \psi^{(0)}_0 \xi >$$

$$\sigma_a^\xi = \frac{1}{k_{\text{eff}}} - \overrightarrow{\nu}^\xi$$

The coefficients of the last two terms in Eq. (26) — the drift term and source (or sink) term — are

$$\overrightarrow{\Gamma}_1^\xi = \frac{1}{N^\xi_i} \left[ \begin{array}{c} - < \sqrt{1 - \mu^2 (\cos \phi_{\text{c}} + \sin \phi_{\text{c}}) \psi^{(0)}_0 \xi, \xi > - \frac{\phi_{\text{c}}}{\partial_{\phi_{\text{c}}}} \psi^{(0)}_0 \xi, \mu_f^\xi > \\ + < \psi^{(0)}_0 \xi, \sqrt{1 - \mu^2 \cos \phi (f^\xi + \theta^\xi)} > - \frac{1}{k_1^\xi} < \psi^{(0)}_0 \xi, \nu_{\sigma_f} \sigma_f^\xi > \end{array} \right]$$

$$\overrightarrow{\Gamma}_2^\xi = \frac{1}{N^\xi_i} \left[ \begin{array}{c} - < \sqrt{1 - \mu^2 (\cos \phi_{\text{c}} + \sin \phi_{\text{c}}) \psi^{(0)}_0 \xi, \xi > - \frac{\phi_{\text{c}}}{\partial_{\phi_{\text{c}}}} \psi^{(0)}_0 \xi, \mu_g^\xi > \\ + < \psi^{(0)}_0 \xi, \sqrt{1 - \mu^2 \sin \phi (f^\xi + \theta^\xi)} > - \frac{1}{k_2^\xi} < \psi^{(0)}_0 \xi, \nu_{\sigma_f} \sigma_f^\xi > \end{array} \right]$$
\[ T^\xi = \frac{1}{N_T} \left[ -\langle \sqrt{1-\mu^2 \cos \phi_G} + \frac{\sin \phi_G}{\sqrt{1-\mu^2}} \rangle \psi^{(0)} \xi, \mu \xi > - \langle \frac{\phi}{\phi_G} \psi^{(0)} \xi, \mu \xi > \right. \\
\left. + \langle \psi^{(0)} \xi, \mu (f \xi \xi + g \xi \xi + h \xi \xi - q \xi) > \frac{1}{k_i^2} < \psi^{(0)} \xi, \nu \sigma_j \xi \xi > \right] , \] (31)

and

\[ S^\xi = \frac{1}{N_T} \left[ \langle \psi^{(0)} \xi, (\sqrt{1-\mu^2 \cos \phi_G} + \frac{\sin \phi_G}{\sqrt{1-\mu^2}}) (f \xi \xi \xi + g \xi \xi \xi + h \xi \xi \xi - q \xi) > \frac{1}{k_i^2} < \psi^{(0)} \xi, \nu \sigma_j \xi \xi \xi \xi > \right] . \] (32)

Finally, transforming Eq. (26) back to dimensional variables yields

\[ \nabla_x \cdot \mathbf{D}^\xi \nabla_x A_0(\xi) + \left( \frac{1}{k_{eff}} \nu \Sigma_f - \Sigma_s \right) A_0(\xi) + \Gamma^\xi \cdot \nabla_x A_0(\xi) + S^\xi A_0(\xi) = 0 \] (33)

where the homogenized diffusion tensor is

\[
\mathbf{D}^\xi = \frac{1}{N_T} \left[
\begin{array}{ccc}
< \psi^{(0)} \xi, \sqrt{1-\mu^2} \cos \phi > & < \psi^{(0)} \xi, \sqrt{1-\mu^2} \cos \phi > & 0 \\
< \psi^{(0)} \xi, \sqrt{1-\mu^2} \sin \phi > & < \psi^{(0)} \xi, \sqrt{1-\mu^2} \sin \phi > & 0 \\
0 & 0 & < \psi^{(0)} \xi, \mu h >
\end{array}\right]
\]

the homogenized cross sections are

\[ \nu \Sigma_f = \frac{1}{N_T} \left[ \psi^{(0)} \xi, \nu \Sigma_f(\xi) \psi^{(0)} \xi > \right. \]

\[ \Sigma_s = \frac{1}{k_{eff}} \nu \Sigma_f \xi \]

the coefficient of the drift term is

\[ \Gamma^\xi = \xi \xi \xi \xi , \]

and the coefficient of the source (or sink) term is

\[ S^\xi = \xi \xi \xi \xi . \]
The overbars on the nuclear parameters indicate that they are assembly-homogenized, i.e. in this equation, the final global equation, they are constant after the averaging within each fuel assembly and have piecewise constant variation over the core. The drift term and the source (or sink) term in Eq. (33), which do not exist in the conventional diffusion equation, but appeared in Part I on the development of the DEB/SHT\(^1\) and in a homogenization theory developed for near-periodic lattice cells\(^5\), are due to the parametric dependence of the cross sections upon the slow scale variable \(\bar{\zeta}\). These source and drift terms which are identically zero for a system comprised of exactly periodic assemblies, provide "corrections" to the leakage between adjacent assemblies, which is not included in the unit homogenization calculations of the heterogeneous assemblies.

It follows from the above development that, to leading order in the small parameter \(\epsilon\), the asymptotic solution to the heterogeneous reactor transport equation is

\[
\psi(\vec{r}, \vec{\Omega}) = A_0(\vec{r})\psi^{(0)}(x, y, \Omega) + O(\epsilon) ,
\]

where \(\psi^{(0)}(x, y, \Omega)\), the solution to Eq. (5), is the rapidly varying unit heterogeneous assembly fundamental eigenfunction of the transport equation and \(A_0(\vec{r})\), the solution to Eq. (33), is the assembly-homogenized global diffusion equation fundamental eigenfunction. The leading order solution given by Eq. (34) naturally provides a self-consistent de-homogenization procedure for the reconstruction of the local heterogeneous transport theory flux from the solutions to the assembly-homogenized global diffusion equation, Eq. (33) (which is solved for \(1/k_{eff}\) and \(A_0(\vec{r})\)) and the heterogeneous assembly transport equation, Eq. (5) (which is solved for \(\psi^{(0)}(x, y, \Omega)\)).
3 Assembly Interface Conditions and Discontinuity Factors

To solve the assembly-homogenized global diffusion equation, Eq. (33), for $A_0(\bar{r})$ using assembly-size meshes, the homogenized-assembly interface conditions must be known. In the transport-equation-based systematic homogenization theory developed in this work, these assembly interface conditions for the assembly-homogenized global diffusion equation arise consistently from the theoretical development by requiring continuity of heterogeneous angular flux at assembly interfaces. Integration of the resulting zeroth order continuity condition at fuel assembly interfaces over all $\hat{\bar{r}}$ yields

$$A_0^+ \psi^{(0),\hat{\bar{r}}}^- = A_0^- \psi^{(0),\hat{\bar{r}}}^+ + O(\epsilon). \tag{35}$$

Here, the minus(-) sign indicates the limit from the left to an interface between two adjacent fuel assemblies and the plus(+) sign indicates the limit from the right. Due to their parametric dependence on variable $\bar{r}$, the fundamental assembly eigenfunctions for adjacent assemblies, $\psi^{(0),\hat{\bar{r}}}^-$ and $\psi^{(0),\hat{\bar{r}}}^+$, are different in general; therefore $A_0(\bar{r})$ must have a finite jump (or flux discontinuity) across homogenized fuel assembly interfaces. This flux discontinuity factor for $A_0(\bar{r})$ naturally follows from the above equation

$$\frac{A_0^+}{A_0^-} = \frac{\psi^{(0),\hat{\bar{r}}}^-}{\psi^{(0),\hat{\bar{r}}}^+} + O(\epsilon), \tag{36}$$

which is used in the coarse-mesh assembly-homogenized global diffusion calculations to solve for $A_0(\bar{r})$. 
Like the discontinuity factors obtained in Part I for the DEB/SHT, these discontinuity factors are space dependent. However, in practical nodal diffusion calculations using zeroth-order nodal methods and assembly-size meshes, surface-averaged discontinuity factors are used on the assembly interfaces. In a two-dimensional calculation with assembly sizes $2a \times 2b$, for instance, the surface-averaged assembly fluxes $\mathcal{A}_0(\pm b) = \frac{1}{a} \int_a^b A_0(x, \pm b)\,dx$ and $\mathcal{B}_0(\pm a) = \frac{1}{b} \int_b^a A_0(\pm a, y)\,dy$ are computed, rather than space-dependent assembly surface fluxes. Therefore, surface-averaged flux discontinuity factors must be introduced on the assembly interfaces in practical nodal calculations. As in Part I on the DEB/SHT, approximate surface-averaged discontinuity factors are generated by simply averaging both sides of Eq. (35) over an assembly interface. Upon expansion of the slowly varying global flux $A_0$ over a node surface, one sees that the linear term in the expansion integrates to zero when multiplied by a symmetric assembly eigenfunction. Such eigenfunctions result for symmetric assemblies such as those loaded with fresh fuel and the assemblies in all the core models studied here. Hence, the node surface averages in Eq. (35) will become the constant (average) value of the $A_0$ times the average of the corresponding $\psi^{(0)}_r$, plus an error term that is second order in the assembly dimension. This dimension is typically about a tenth the characteristic core dimension for a light water reactor; thus, the error will be about 0.01 which is comparable to the error that already appears in the leading order solution given by Eq. (34) since $\epsilon$, the ratio of the total mean free path to the core dimension also is about 0.01. Hence, after expansion of the $A_0$ on the interface and integration over that interface, Eq. (35) for the interface at $y = \pm b$ between a pair of two-dimensional assemblies, becomes
\[
A_0^{x,+}(\pm b) \overline{\psi}^{x,(0),x,+}(\pm b) = A_0^{x,-}(\pm b) \overline{\psi}^{x,(0),x,-}(\pm b) + O(\varepsilon),
\]

where
\[
\overline{\psi}^{x,(0),x}(\pm b) = \frac{1}{2a} \int_z \overline{\psi}^{x,(0),x}(x, \pm b) dx,
\]

and the overbar-x on \( A_0 \) and \( \overline{\psi}^{x,(0),x} \) indicate the surface average. It follows that the approximate discontinuity factors at the top and bottom surfaces are
\[
\frac{A_0^{x,+}(\pm b)}{A_0^{x,-}(\pm b)} = \frac{\overline{\psi}^{x,(0),x,-}(\pm b)}{\overline{\psi}^{x,(0),x,+}(\pm b)} + O(\varepsilon). \tag{37}
\]

Similarly, Eq. (35) after expansion of the \( A_0 \), is integrated over \( y \) along an assembly interface to yield
\[
A_0^{x,+}(\pm a) \overline{\psi}^{x,(0),x,+}(\pm a) = A_0^{x,-}(\pm a) \overline{\psi}^{x,(0),x,-}(\pm a) + O(\varepsilon),
\]

where \( \overline{\psi}^{x,(0),x}(\pm a) = \frac{1}{2a} \int_y \overline{\psi}^{x,(0),x}(\pm a, y) dy \) are the heterogeneous surface-averaged fluxes from the unit heterogeneous assembly calculations, and the flux discontinuity factors on the right and left surfaces of the homogenized assemblies are
\[
\frac{A_0^{x,+}(\pm a)}{A_0^{x,-}(\pm a)} = \frac{\overline{\psi}^{x,(0),x,+}(\pm a)}{\overline{\psi}^{x,(0),x,-}(\pm a)} + O(\varepsilon). \tag{38}
\]

4 Local Flux and Pin Power Reconstruction

In practical coarse-mesh nodal calculations assembly-size nodes are normally used. Thus, as stated in the previous section, only node-averaged (therefore, normally assembly-averaged) fluxes and node surface-averaged partial or net currents are obtained in zeroth-order nodal methods.\(^6\) Hence, in order to calculate the pin power, the
local heterogeneous flux must be reconstructed. The development of the transport-
equation-based systematic homogenization theory presented above naturally provides
a self-consistent procedure by which for the reconstruction of these local fluxes; by
simply multiplying each of the homogenized assembly fluxes that are calculated in
the global calculation — done via the assembly-homogenized diffusion equation, Eq.
(33) — by the corresponding heterogeneous-assembly eigenfunction, the leading or-
der for the heterogeneous-system flux given by Eq. (34) is reconstructed. However,
the assembly-averaged fluxes that result from a zeroth-order nodal method solution
of the global diffusion equation, carried out using assembly size nodes as usually is
done in practice, does not have adequate space dependence within the assemblies to
yield accurate reconstructed local fluxes. Hence, for accurate reconstruction some
global space dependence of the fluxes within the assemblies is necessary. Since Eq.
(34) does not require that $\phi_0(r)$ be taken directly from the coarse-mesh nodal cal-
culation but rather that a good solution to the global diffusion be used, a better
approach, which was introduced in Part I for the DEB/SHT,1 is to obtain good
space-dependent fluxes within the homogenized assemblies and use them in the re-
construction procedure. These space-dependent node-interior fluxes are available,
usually through quadratic terms,7 directly from the global calculation, if a higher or-
der nodal method7 is used. However, if the space dependence of the fluxes within the
homogenized assemblies is needed following a less costly zeroth-order nodal calcula-
tion, it must be determined in some way from the results of the calculation. This can
be done by simply using as boundary conditions the final converged net currents from
the quadratic transverse fits used in the global nodal diffusion calculation and solving
the resulting local boundary value problem for each assembly. Using these net currents on surfaces as boundary conditions, the Green's functions for the homogenized assemblies can be conveniently employed to solve the local boundary value problem and determine the assembly-interior space-dependence of the global flux $A_0(r)$. The resulting expressions for $A_0(r)$ within each assembly conserve the assembly leakages calculated in the global coarse-mesh nodal calculation. For the two-dimensional case, this space-dependent global flux within a homogenized assembly of volume $(-a,+a)$ is given by

$$A_0(x,y) = \int_{-a}^{a} dx_0 \left[ G(x,y|x_0,-b)J(x_0,-b) + G(x,y|x_0,b)J(x_0,b) \right]$$

$$+ \int_{-b}^{b} dy_0 \left[ G(x,y|-a,y_0)J(-a,y_0) + G(x,y|a,y_0)J(a,y_0) \right], \quad (39)$$

where the calculated net currents on the assembly (node) surfaces provide $J'$s and $G(x,y|\alpha_0,\gamma_0)$ is the Green's function for the assembly-homogenized diffusion equation with homogeneous Neumann boundary conditions. In order to insure diagonal symmetry for a node with symmetric boundary conditions, this Green's function is written in terms of both the $x$- and $y$-eigenfunctions as

$$G(x,y|x_0,\gamma_0) = \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} \frac{f_n(x)\gamma_k(y)J_n(x_0)\gamma_k(y_0)}{N_{n,k}}, \quad (40)$$

where

$$f_n(x) = \begin{cases} 
\sin\beta_n x, & \beta_n = \frac{\pi n}{2a}, \quad n = 1,3,5,... \\
\cos\beta_n x, & \beta_n = \frac{\pi n}{2a}, \quad n = 0,2,4,... 
\end{cases}$$

$$g_k(y) = \begin{cases} 
\sin\gamma_k y, & \gamma_k = \frac{\pi k}{2b}, \quad k = 1,3,5,... \\
\cos\gamma_k y, & \gamma_k = \frac{\pi k}{2b}, \quad k = 0,2,4,... 
\end{cases}$$
NODAL DIFFUSION METHODS. II

\[ N_{n,k} = \mathcal{D}(k^2 - \beta_n^2 - \gamma_k^2)(a - (-1)^n \frac{\sin(2\beta_n a)}{2\beta_n})(b - (-1)^k \frac{\sin(2\gamma_k b)}{2\gamma_k}) \]

and \( k^2 = \frac{1}{\Sigma_{eff}/\nu_\Sigma_f - \Sigma_a}/\mathcal{D} \). The local reconstructed heterogeneous fluxes thus are obtained according to Eq. (34) by multiplying the resulting space-dependent diffusion theory flux \( A_0(x,y) \) within a homogenized assembly by the fundamental assembly transport theory eigenfunction \( \psi^{(0)}_{\text{as}}(x,y,\hat{n}) \). The pin powers then are calculated easily from these reconstructed or "de-homogenization" transport theory fluxes.

5 Implementation

There are three steps in each numerical calculation carried out within the framework of this new transport-equation-based systematic homogenization theory (TEB/SHT). They are: the homogenization of the heterogeneous assemblies using a nodal transport calculation to solve the transport equation for each type assembly; the solution to the assembly-homogenized global diffusion equation via a coarse-mesh nodal diffusion calculation; and the reconstruction of the local heterogeneous transport theory flux.

In the first step, the discrete nodal transport method (DNTM)\(^8\) was used with fine-mesh lattice-cell-size nodes to obtain assembly-homogenized parameters via an eigenvalue calculation with periodic boundary conditions for each type fuel assembly to determine the fuel assembly fundamental eigenfunction \( \psi^{(0)}_{\text{as}} \), which then was used to generate the quantities to be used in the global coarse-mesh nodal diffusion calculation or in the subsequent local flux reconstruction. These were: the assembly-homogenized cross-sections, the normalized surface-averaged assembly fluxes used to produce the assembly interface flux discontinuity factors for the global diffusion
calculation; and the normalized assembly fluxes (or form functions)—the eigenfunctions themselves—used in the local heterogeneous flux reconstruction. The eigenfunctions from the heterogeneous assembly calculations were normalized so that their assembly averages were unity. (Therefore the surface averages of these eigenfunctions are identical to the “assembly discontinuity factors” (ADFs) in generalized equivalence theory). Hence, after the eigenvalue calculation was completed, fixed-source calculations with periodic boundary conditions were done for the same assemblies to calculate the functions \( f^\xi(\xi_1, \xi_2, \Omega) \) and \( g^\xi(\xi_1, \xi_2, \Omega) \) using Eqs. (16) and (17). These functions are needed along with the assembly eigenfunctions to construct the assembly-homogenized diffusion tensor. Convergence criteria for the eigenvalue calculations and the fixed-source calculations were \( 10^{-12} \) and \( 10^{-10} \), respectively. Very tight convergence criteria were necessary on the eigenfunction calculations. Because the homogeneous form of Eqs. (16) and (17) has a solution (the assembly eigenfunction), \( f^\xi(\xi_1, \xi_2, \Omega) \) and \( g^\xi(\xi_1, \xi_2, \Omega) \) were calculated as generalized inverses and errors in the source terms which are orthogonal to the assembly adjoint eigenfunction would lead to a contribution that is not orthogonal to that eigenfunction and cause the iterative solution procedure to diverge if those errors are not very small. The derivatives with respect to the slow-scale variable \( \zeta \), which are small but in general not zero, were taken to be zero in the assembly calculations reported here. Thus \( \frac{1}{\xi_1} \) and the drift term and the source (or sink) term coefficients in Eq. (33) were zero.

After the assembly-homogenized parameters were determined, they were used along with the flux discontinuity factors—the ratios of the limits of the surface averages of the heterogeneous assembly normalized eigenfunctions from opposite sides
of the interfaces between adjacent assemblies — in the second step of the calculation, the nodal Green's function method (NGFM)\textsuperscript{10} coarse-mesh global diffusion calculation with one node per assembly, to compute the node-averaged (assembly-averaged) fluxes and the reactor eigenvalue. The convergence criterion for the coarse-mesh NGFM global diffusion calculation was 10\textsuperscript{-10}.

Finally, after the global coarse-mesh nodal diffusion calculation, in the third step the local heterogeneous fluxes were reconstructed by multiplying the local heterogeneous assembly form functions $\psi^{(0),h}$ determined in step 1, by the homogenized assembly fluxes $A_0$. As discussed above in Sec. 4, the space dependence of homogenized assembly fluxes was obtained via Eq. (39).

The results of the computations based on the TEB/SHT, carried out as just described, were compared with reference solutions obtained via global fine-mesh heterogeneous DNTM calculations with the fine mesh size the same as that used in the unit assembly calculations, i.e. one node per fuel lattice cell. These results also were compared with those obtained via coarse-mesh nodal diffusion calculations done using generalized equivalence theory (GET) parameters.

As was discussed in Part I on the diffusion-equation-based theory,\textsuperscript{1} when the assemblies are \textit{internally symmetric}, as is the case in all the test problems studied here, the periodic boundary conditions on the assembly eigenfunctions can be recast in somewhat more convenient form. This internal symmetry of the assemblies also causes $D_{12}^{V}$ and $D_{21}^{V}$ to be identically zero, and the assembly-homogenized global diffusion equation, Eq. (33), takes on the conventional form of the diffusion equation, but of course with TEB/SHT homogenized parameters.
Using the three steps in the procedure described above, several test problems were studied to evaluate the transport-equation-based/systematic-homogenization-theory. The results are presented in the next section.

6 Numerical Results

The first test problem is a simple, one-dimensional problem that was solved to validate the TEB/SHT. It has the same geometry as the first test problem studied in Part I to validate the DEB/SHT developed there. It has similar nuclear data, but it is not identical since a diffusion coefficient formed part of the data there. It is a symmetric slab reactor with two water reflectors, each of the same width as an assembly, and a core comprised of twelve near-periodic assemblies of two types (A and B). In each assembly there are three regions, one 1.0 cm central region flanked by two 10.0 cm identical fuel regions. The 1.0 cm central regions in assembly types A and B contain water and poison, respectively. The basic nuclear parameters of the materials in these assemblies are tabulated in Table 1, and the assembly-homogenized parameters that were obtained via 21 node, S-16, DNTM calculations, are given in Table 2, along with the flux discontinuity factors at the assembly interfaces. Global NGFM calculations with one node per assembly were carried out both within the TEB/SHT framework and using the GET procedure to solve the assembly-homogenized global diffusion equation. Eigenvalues from these coarse-mesh NGFM calculations with and without flux discontinuity factors are compared in Table 3 with the eigenvalue obtained from the fine-mesh whole-reactor solution of the transport equation obtained
Table 1: Basic nuclear parameters for the one-dimensional test problem.

<table>
<thead>
<tr>
<th></th>
<th>$\Sigma_T$</th>
<th>$\Sigma_e$</th>
<th>$\nu \Sigma_f$</th>
<th>$\Sigma_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel</td>
<td>1.000</td>
<td>0.066</td>
<td>0.070</td>
<td>0.934</td>
</tr>
<tr>
<td>Water</td>
<td>3.472</td>
<td>0.010</td>
<td>0.000</td>
<td>3.462</td>
</tr>
<tr>
<td>Poison</td>
<td>2.500</td>
<td>0.040</td>
<td>0.000</td>
<td>2.460</td>
</tr>
</tbody>
</table>

Table 2: Assembly-homogenized parameters for the one-dimensional test problem.

<table>
<thead>
<tr>
<th></th>
<th>$D$</th>
<th>$\Sigma_e$</th>
<th>$\nu \Sigma_f$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Assembly A</td>
<td>SHT</td>
<td>0.2938790206</td>
<td>0.06364916818</td>
</tr>
<tr>
<td>Assembly B</td>
<td>FVV</td>
<td>0.3226569018</td>
<td>0.06248077678</td>
</tr>
<tr>
<td>Assembly B</td>
<td>SHT</td>
<td>0.2926383099</td>
<td>0.06551973387</td>
</tr>
<tr>
<td>Assembly B</td>
<td>FVV</td>
<td>0.32569013711</td>
<td>0.06499484491</td>
</tr>
<tr>
<td>Discontinuity Factor (A/B)</td>
<td></td>
<td>1.0268430490</td>
<td></td>
</tr>
</tbody>
</table>

Table 3: Comparison of the computed eigenvalues for the one-dimensional test problem.

<table>
<thead>
<tr>
<th></th>
<th>$k_{\text{eff}}$</th>
<th>Percent Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fine-Mesh DNTM</td>
<td>1.04663820</td>
<td>—</td>
</tr>
<tr>
<td>C-M GET Diff. W/O DF</td>
<td>1.04612846</td>
<td>-0.0487%</td>
</tr>
<tr>
<td>C-M TEB/SHT Diff. W/O DF</td>
<td>1.04632551</td>
<td>-0.0300%</td>
</tr>
<tr>
<td>C-M GET Diff. W/ DF</td>
<td>1.04638062</td>
<td>-0.0246%</td>
</tr>
<tr>
<td>C-M TEB/SHT Diff. W/ DF</td>
<td>1.04657219</td>
<td>-0.0063%</td>
</tr>
</tbody>
</table>

via a 294-node S-16 DNTM calculation. Assembly powers were calculated using assembly-homogenized nuclear parameters with discontinuity factors both within the TEB/SHT framework and using the GET procedure, and the results are shown in Table 4 for the six assemblies to the right of the symmetry plane. These results show that, for both the TEB/SHT based calculations and the GET based calculations, introducing flux discontinuity factors improved the computed reactor eigenvalue (Table 3) and assembly powers (Table 4). When the discontinuity factors were used in
conjunction with TEB/SHT parameters, the percent error in $k_{eff}$ was $-0.0063\%$, the maximum assembly power error was $-2.264\%$, and the fractional $L_1$ (power) error was $1.500\%$. By comparison, when they were used in conjunction with GET parameters, the percent errors were $-0.024656$, $9.859\%$ and $3.641\%$, respectively. Thus, TEB/SHT parameters clearly led to a more accurate eigenvalue and more accurate assembly powers than the GET parameters for this simple test problem.

Reconstruction of the local heterogeneous fluxes followed step 3 in section 5; the space-dependent homogenized assembly fluxes from the global coarse-mesh NGFM diffusion calculation, carried out within the TEB/SHT framework, were multiplied by the heterogeneous assembly form functions, i.e. by the normalized angular fluxes from the heterogeneous unit assembly fine-mesh, S-16, DNTM calculations. The space-dependent flux within homogenized assemblies was obtained by solving the diffusion equation in homogenized assemblies analytically with net currents, computed in the coarse-mesh TEB/SHT calculation, as the boundary conditions.

Assembly powers computed using reconstructed fluxes — which have a fractional $L_1$ error of $1.456\%$ — also are presented in Table 4. The errors in the reconstructed

---

Table 4: Comparison of assembly powers from coarse-mesh NGFM diffusion calculations using TEB/SHT framework and GET procedure with those from a fine-mesh, DNTM (S-16) calculation for the one-dimensional test problem.

<table>
<thead>
<tr>
<th>No.(type) of assembly</th>
<th>F-M DNTM Power</th>
<th>C-M SHT W/ DF Error(%)</th>
<th>C-M GET W/ DF Error(%)</th>
<th>Recon. Power Error(%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 (A)</td>
<td>2.3968779</td>
<td>1.269</td>
<td>-3.097</td>
<td>1.235</td>
</tr>
<tr>
<td>2 (B)</td>
<td>1.3940750</td>
<td>-2.079</td>
<td>-2.511</td>
<td>-2.018</td>
</tr>
<tr>
<td>3 (A)</td>
<td>1.0640932</td>
<td>0.999</td>
<td>3.426</td>
<td>0.966</td>
</tr>
<tr>
<td>4 (B)</td>
<td>0.5896319</td>
<td>-2.264</td>
<td>3.498</td>
<td>-2.203</td>
</tr>
<tr>
<td>5 (A)</td>
<td>0.3997440</td>
<td>0.984</td>
<td>9.208</td>
<td>0.950</td>
</tr>
<tr>
<td>6 (B)</td>
<td>0.1555780</td>
<td>-1.712</td>
<td>9.859</td>
<td>-1.650</td>
</tr>
</tbody>
</table>
assembly powers are slightly smaller than those in the assembly powers calculated directly in the coarse-mesh NGFM calculation using TEB/SHT parameters. Figure 1 shows the reconstructed scalar fluxes for this one-dimensional test problem. The dips in the curves occur where the poison regions are located. Based on various additional test problems not reported here, it was observed that errors in the reactor eigenvalue and in the assembly power distribution, calculated using the coarse-mesh NGFM within the TEB/SHT framework, increased with increasing absorption cross sections in the poison or control rod region (which consequently moves flux discontinuity factors further from unity). These results are consistent with the fact that the TEB/SHT is developed for near-periodic systems, and the system is moved further from periodic as the absorption in the poison regions is increased.

The second problem is a small two-dimensional PWR model. It has the geometric structure as the second problem used in Part I to evaluate the diffusion-equation-based/SHT, except the outer part of the water reflector forms a square here; the nuclear data is similar, but not identical. It consists of a water reflector (R) and a core comprised of 69 assemblies of three types: assemblies with fresh fuel pins and water holes (E1); assemblies with partially burned fuel pins and water holes (E2); and assemblies with fresh fuel pins and control rods (C).

Each assembly (see Fig. 2) is 12 cm x 12 cm and contains 64 (8x8) homogeneous lattice cells, four of which are control rods or water holes. The basic nuclear data is given in Table 5. The assembly-homogenized nuclear parameters and the assembly interface flux discontinuity factors obtained for each type of assembly using 8 x 8 mesh, S-4, DNTM (transport) calculations are given in Table 6. Taking advantage of
Figure 1: Comparison between the local fluxes reconstructed from the coarse-mesh global NGFM calculation, done within the TEB/SHT framework, and the fine-mesh DNTM (S-16) calculation flux, for the one-dimensional test problem.

Figure 2: Fuel assembly geometry for the small PWR model: (I) control rods/water holes; (II) fuel pins.
Table 5: Nuclear parameters for the small two-dimensional PWR model.

<table>
<thead>
<tr>
<th>Nuclear Parameters</th>
<th>Fresh Fuel</th>
<th>Partially Burned Fuel</th>
<th>Water</th>
<th>Control Rod</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Sigma_f$</td>
<td>0.360</td>
<td>0.360</td>
<td>0.900</td>
<td>0.480</td>
</tr>
<tr>
<td>$\Sigma_e$</td>
<td>0.140</td>
<td>0.142</td>
<td>0.010</td>
<td>0.300</td>
</tr>
<tr>
<td>$\nu\Sigma_f$</td>
<td>0.150</td>
<td>0.147</td>
<td>0.000</td>
<td>0.000</td>
</tr>
</tbody>
</table>

Table 6: Assembly-homogenized parameters for the small two-dimensional PWR model.

<table>
<thead>
<tr>
<th>Type of Assemblies</th>
<th>$D$</th>
<th>$\Sigma_e$</th>
<th>$\nu\Sigma_f$</th>
</tr>
</thead>
<tbody>
<tr>
<td>E1 (Fresh Fuel + Water)</td>
<td>0.8575939637</td>
<td>0.1320562403</td>
<td>0.1408258880</td>
</tr>
<tr>
<td></td>
<td>0.8915757314</td>
<td>0.1319620545</td>
<td>0.1407254475</td>
</tr>
<tr>
<td>(P. B. Fuel + Water)</td>
<td>0.8575939637</td>
<td>0.133939188</td>
<td>0.1380093703</td>
</tr>
<tr>
<td>E2</td>
<td>0.8915757314</td>
<td>0.1338383938</td>
<td>0.1379109385</td>
</tr>
<tr>
<td>C</td>
<td>0.8983560815</td>
<td>0.1500633009</td>
<td>0.1450218549</td>
</tr>
<tr>
<td>(Fresh Fuel + Poison)</td>
<td>0.9147529764</td>
<td>0.1477227427</td>
<td>0.1427599287</td>
</tr>
<tr>
<td>Discontinuity Factors</td>
<td>E1/C = 1.0035181418/1.084164442</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>E2/C = 1.0035181418/1.0841674442</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

the quarter-core symmetry, the assembly-homogenized global diffusion equation was solved for a quarter core using one node per assembly, i.e. a total of 121 nodes for the full core (69 assemblies and 52 assembly-size nodes in the reflector), both within the TEB/SHT framework and using the GET procedure. Both calculations were carried out both with and without discontinuity factors incorporated into the NGFM. The reference solution was obtained via a fine-mesh 64-equal-size-nodes per assembly, S-4, DNTM transport calculation, i.e. a total of 7744 nodes.

Comparison of the results with the reference solution show that the coarse-mesh NGFM calculations yielded a better reactor eigenvalue and assembly power distribution both with the TEB/SHT parameters and with the GET parameters when the discontinuity factors were included. The eigenvalues of the coarse-mesh NGFM
calculations using the TEB/SHT parameters and the GET parameters, with discontinuity factors, are compared in Table 7, and the corresponding powers are compared in Table 8. The 11 x 11 TEB/SHT calculation yielded an error of \(-0.060\%\) in \(k_{\text{eff}}\), a maximum error of 2.30\% in assembly power, and a fractional \(L_1\) error of 0.41\% in assembly power, while the 11 x 11 GET-based calculation yielded \(-0.068\%, 5.73\%\) and 1.63\%, respectively, for these quantities. Clearly, the TEB/SHT parameters led to more accurate results than the GET parameters.

As for the simple one-dimensional problem, the local heterogeneous fluxes were reconstructed by multiplying the assembly fundamental eigenfunction by the spatial variation of fluxes within homogenized assemblies [Eq. (34)]. The space dependence of the fluxes within the homogenized assemblies was obtained using the Green's functions with the quadratically fitted net currents on homogenized assembly surfaces, as described in Section 4. These reconstructed fluxes were then used to calculate the pin powers, and the assembly powers were recalculated from them. These assembly powers, calculated from the reconstructed fluxes, also are presented in Table 8. They yielded a fractional \(L_1\) error of 0.66\% which is larger than the 0.41\% value for the \(L_1\) assembly power error that resulted from the original TEB/SHT-based coarse-mesh NGFM calculation. The corresponding assembly powers calculated from the reconstructed fluxes also have errors that are larger in most assemblies than those of the powers calculated directly in the NGFM, as is clear from Table 8. In Fig. 3 the reconstructed fluxes are compared with the fine-mesh S-4 DNTM calculation fluxes in the four rows of pins just above the middle symmetry plane and parallel to the \(x\)-axis. The agreement is excellent. The dips in the second row are due to the control rods at those locations.
Table 7: Reactor eigenvalue for the small PWR model.

<table>
<thead>
<tr>
<th></th>
<th>$k_{eff}$</th>
<th>Percent Errors</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fine-Mesh DNTM</td>
<td>1.02631088</td>
<td>——</td>
</tr>
<tr>
<td>GET W/ DF</td>
<td>1.02552293</td>
<td>-0.068</td>
</tr>
<tr>
<td>TEB/SHT W/ DF</td>
<td>1.02571875</td>
<td>-0.060</td>
</tr>
</tbody>
</table>

Table 8: Assembly powers for the small PWR model.

<table>
<thead>
<tr>
<th>E2</th>
<th>E2</th>
<th>E2</th>
<th>— Assembly Type</th>
<th>— Fine-Mesh DNTM</th>
<th>— C-M GET % Error</th>
<th>— C-M TEB/SHT % Error</th>
<th>— Recon. Power % Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5047</td>
<td>0.4338</td>
<td>0.3305</td>
<td>E2</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>3.21</td>
<td>4.49</td>
<td>5.73</td>
<td>El</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>0.39</td>
<td>1.37</td>
<td>1.86</td>
<td>El</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>0.80</td>
<td>1.78</td>
<td>2.28</td>
<td>El</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>E1</td>
<td>C</td>
<td>E2</td>
<td>E2</td>
<td>1.02631088</td>
<td>—0.068</td>
<td>1.02552293</td>
<td>—0.060</td>
</tr>
<tr>
<td>0.9575</td>
<td>0.7398</td>
<td>0.5894</td>
<td>C</td>
<td>1.4928</td>
<td>1.6000</td>
<td>0.9481</td>
<td>0.5894</td>
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</tr>
<tr>
<td>E1</td>
<td>E1</td>
<td>E1</td>
<td>E1</td>
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<td>2.4262</td>
<td>1.4928</td>
<td>0.9481</td>
</tr>
<tr>
<td>2.5445</td>
<td>2.4262</td>
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</tr>
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<td>-1.18</td>
<td>-1.16</td>
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<td>E1</td>
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<td>—</td>
<td>—</td>
</tr>
<tr>
<td>-0.27</td>
<td>-0.14</td>
<td>-0.14</td>
<td>E1</td>
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<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>0.02</td>
<td>0.13</td>
<td>0.14</td>
<td>E1</td>
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<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>E1</td>
<td>E1</td>
<td>E1</td>
<td>E1</td>
<td>2.3212</td>
<td>2.5445</td>
<td>1.4928</td>
<td>0.9481</td>
</tr>
<tr>
<td>2.3212</td>
<td>2.5445</td>
<td>1.4928</td>
<td>E1</td>
<td>—</td>
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<td>—</td>
</tr>
<tr>
<td>-2.48</td>
<td>-1.18</td>
<td>-1.57</td>
<td>E1</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
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<tr>
<td>-0.41</td>
<td>-0.27</td>
<td>-0.39</td>
<td>E1</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>-1.09</td>
<td>0.02</td>
<td>-1.07</td>
<td>E1</td>
<td>—</td>
<td>—</td>
<td>—</td>
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</tr>
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</table>
Figure 3: Comparison of reconstructed local flux with reference flux from a fine-mesh (pin-size mesh) DNTM (S-4) calculation of the four rows of pins above the middle symmetry plane and parallel to the x-axis of the small PWR model.

The third test problem is a large two-dimensional PWR benchmark model. Its geometry is the same as to that of the large PWR model used in Part I except the outer part of the water reflector forms a square here; and the nuclear data is similar, but not identical. The geometric description is repeated here for completeness. It is comprised of a water reflector (R) and a complex core with 193 assemblies of five types: assemblies with fresh fuel pins and water holes (E1), assemblies with
partially burned fuel pins and water holes (E2), assemblies with spiked fuel pins and water holes (E3), assemblies with fresh fuel pins and control rods (C1), and assemblies with partially burned fuel pins and control rods (C2). The reactor core has quarter-core symmetry about the center of the middle assembly. The assembly geometry is shown in Fig. 4. The nuclear data is given in Table 9, and the assembly-homogenized nuclear parameters and flux discontinuity factors obtained via a 256-equal-size-node per assembly S-4, DNTM transport calculation are given in Table 10. The assembly-homogenized global diffusion equation was solved in a quarter core both with TEB/SHT and GET parameters using assembly-size meshes, i.e. a total of 17x17 nodes in the full core (193 assemblies and 96 assembly-size-nodes in the reflector), with discontinuity factors incorporated into the NGFM. The results were compared with the reference solutions obtained using a 256-equal-size-node per assembly S-4, DNTM calculation, i.e. a total of 73,984 nodes. The eigenvalues from the coarse-mesh NGFM calculations done using TEB/SHT parameters and GET parameters, with discontinuity factors are compared in Table 11, and the corresponding assembly powers are compared in Table 12. The 17 x 17 TEB/SHT-based calculation yielded an error of -0.161% in $k_{eff}$, a maximum error of 4.82% in assembly power, and an $L_1$ assembly power error of 1.40%, whereas the 17 x 17 GET-based calculation yielded values of -0.413%, 10.04%, and 2.80%, respectively. Confirming conclusions drawn from the small PWR problem, these coarse-mesh NGFM calculations also showed that the TEB/SHT parameters generated more accurate results than the GET parameters.

Next, using Eq. (34), the local heterogeneous fluxes were reconstructed as described above for the previous test problem, the small PWR problem. The recon-
constructed fluxes then were used to determine the reconstructed pin powers which in turn were used to reconstruct assembly powers. The reconstructed assembly powers (Table 12) yielded a fractional $L_1$ error of 1.43%, slightly higher than the value of 1.40% that resulted from the original TEB/SHT-based coarse-mesh diffusion calculation. The reconstructed pin powers for the four rows of pins just above the middle symmetry plane and parallel to the x-axis are compared with the reference pin powers in Fig. 5. The excellent agreement between the reconstructed pin powers and

Table 9: Nuclear parameters for the large two-dimensional PWR model.

<table>
<thead>
<tr>
<th>Nuclear Parameters</th>
<th>Fresh Fuel</th>
<th>Partially Burned Fuel</th>
<th>Spiked Fuel</th>
<th>Water</th>
<th>Control Rods</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Sigma_T$</td>
<td>0.2474</td>
<td>0.2381</td>
<td>0.2290</td>
<td>0.9000</td>
<td>0.3340</td>
</tr>
<tr>
<td>$\Sigma_e$</td>
<td>0.0208</td>
<td>0.0222</td>
<td>0.0223</td>
<td>0.0100</td>
<td>0.1050</td>
</tr>
<tr>
<td>$\nu \Sigma_f$</td>
<td>0.0264</td>
<td>0.0259</td>
<td>0.0285</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
</tbody>
</table>

Figure 4: Fuel assembly geometry for the large two-dimensional PWR model: (I) control rods/water holes; (II) fuel pins.
Table 10: Assembly-homogenized parameters for the large two-dimensional PWR model.

<table>
<thead>
<tr>
<th>Type of Assemblies</th>
<th>$D$</th>
<th>$\Sigma_a$</th>
<th>$\nu \Sigma_f$</th>
</tr>
</thead>
<tbody>
<tr>
<td>E1 (Fresh Fuel + Water)</td>
<td>SHT</td>
<td>1.154379692</td>
<td>0.02007288503</td>
</tr>
<tr>
<td></td>
<td>FVW</td>
<td>1.271751402</td>
<td>0.02005660292</td>
</tr>
<tr>
<td>E2 (P. B. Fuel + Water)</td>
<td>SHT</td>
<td>1.191115238</td>
<td>0.02127309671</td>
</tr>
<tr>
<td></td>
<td>FVW</td>
<td>1.320330602</td>
<td>0.0215595424</td>
</tr>
<tr>
<td>E3 (Spiked Fuel + Water)</td>
<td>SHT</td>
<td>1.229435143</td>
<td>0.02136525641</td>
</tr>
<tr>
<td></td>
<td>FVW</td>
<td>1.371622695</td>
<td>0.02134815804</td>
</tr>
<tr>
<td>C1 (Fresh Fuel + Poison)</td>
<td>SHT</td>
<td>1.306142602</td>
<td>0.0336395335</td>
</tr>
<tr>
<td></td>
<td>FVW</td>
<td>1.323992658</td>
<td>0.03320686158</td>
</tr>
<tr>
<td>C2 (P. B. Fuel + Poison)</td>
<td>SHT</td>
<td>1.352280390</td>
<td>0.03488195404</td>
</tr>
<tr>
<td></td>
<td>FVW</td>
<td>1.373065308</td>
<td>0.03443615624</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Discontinuity Factors</th>
</tr>
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<tbody>
<tr>
<td>E1/C1 = 1.0048918598/1.0825961324</td>
</tr>
<tr>
<td>E2/C2 = 1.0047839527/1.0805220472</td>
</tr>
<tr>
<td>E3/Reflector = 1.0046772280/1.0</td>
</tr>
</tbody>
</table>

Table 11: Reactor eigenvalue for the large PWR model.

<table>
<thead>
<tr>
<th></th>
<th>$k_{eff}$</th>
<th>Percent Errors</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fine-Mesh DNTM</td>
<td>1.02288762</td>
<td></td>
</tr>
<tr>
<td>GET W/ DF</td>
<td>1.01866686</td>
<td>-0.413</td>
</tr>
<tr>
<td>TEB/SHT W/ DF</td>
<td>1.02123817</td>
<td>-0.161</td>
</tr>
</tbody>
</table>

the reference pin powers shows that the transport-equation-based systematic homogenization theory reported here provides a framework that can be used not only for the accurate calculation of $k_{eff}$ and assembly powers using coarse-mesh nodal methods but also for the accurate reconstruction of pin powers within the assemblies.

7 Summary

A systematic homogenization theory, based on a multiple-scale asymptotic expansion of the neutron transport equation, has been developed. In this development, homog-
Table 12: Assembly powers for the large PWR model.

| E3  | E3     | E3   | E3   | E3   | E3   | E3   | E3   | E3   | E3   | E3   | E3   | E3   | E3   | E3   | E3   | E3   |
|-----|--------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| 0.8064 | 0.8274 | 0.7263 | 0.5943 | 1.43 | 0.99  | 2.13 | 4.01 | 3.05 | 3.15  | 3.35  | 4.41  | 3.13 | 3.23  | 3.43  | 4.49 |
| 2.4544 | -1.93  | -0.17 | -0.08 | E2   | 2.2947 | 5.14  | 3.40  | 5.08  | 5.45  | 8.49  | 0.45  | 3.17  | 1.00  | 3.64  | 4.82  | 4.49 |
| -1.1527 | 1.66   | -0.05 | -1.40 | 0.15  | 3.33  | 0.63  | 3.81  | 4.90  | 4.57  | C1    | 0.8064 | 1.43  | 3.05  | 1.66  | -0.05 | 0.11  |
| 1.1527 | 1.66   | -0.05 | -1.40 | 0.15  | 3.33  | 0.63  | 3.81  | 4.90  | 4.57  | C1    | 0.8064 | 1.43  | 3.05  | 1.66  | -0.05 | 0.11  |
| 2.2947 | 2.4544 | 1.3710 | 0.5441 | 0.9654 | 1.1527 | 1.5935 | 1.3606 | 0.3007 | 0.2149 | 0.3183 | E2   | 0.8274 | 0.3606 | 10.04 | 2.19  | 0.64  | 3.64  |
| -1.11  | -1.93  | 1.19  | 2.70  | 10.04 | 2.19  | 0.64  | 3.64  | 4.49  | C1    | 0.8064 | 1.43  | 3.05  | 1.66  | -0.05 | 0.11  |
| -0.61  | -0.17  | -0.25 | -2.97 | 2.19  | 0.64  | 3.64  | 4.49  | C1    | 0.8064 | 1.43  | 3.05  | 1.66  | -0.05 | 0.11  |
| -0.45  | -0.08  | -0.09 | -3.35 | 2.36  | 0.27  | 3.81  | 4.49  | C1    | 0.8064 | 1.43  | 3.05  | 1.66  | -0.05 | 0.11  |
enized nuclear parameters and corresponding flux discontinuity factors were systematically and self-consistently derived along with the homogenized diffusion equation to be used with these quantities. One- and two-dimensional test problems have been solved via coarse-mesh nodal diffusion calculations carried out within the TEB/SHT framework. The results show that the combination (TEB/SHT and coarse-mesh nodal diffusion method) yields accurate numerical solutions when compared with fine-mesh
reference transport solutions. The higher accuracy of these results in comparison with the results of generalized equivalence theory, which is based on simple flux and volume weighted homogenized parameters, suggests that the TEB/SHT reported here has the potential to offer an appealing alternative to the rather ad hoc generalized equivalence theory. Moreover, the self-consistent local flux reconstruction procedure that results, within the framework of the systematic homogenization theory, makes possible the accurate determination of pin powers from coarse-mesh (assembly size) nodal calculations. The reconstructed pin powers\(^4\) show that they can be determined accurately in all but the lowest power, least important, pins.

The theoretical development presented here began from the one-speed transport equation for a heterogeneous system, and it led to an assembly-homogenized one-speed diffusion equation. The extension of this development to derive multigroup assembly-homogenized diffusion equations, starting from the multigroup transport equations, could be carried out for the case of linearly anisotropic scattering by building on ideas introduced by G. C. Pomraning\(^1\) in his development of one-speed and multigroup diffusion equations as respective asymptotic approximations to the one-speed and multigroup transport equations for spatially uniform systems. There, the terms corresponding to in-scatter from other groups, in the context of radiative transfer, were taken to be small (second order in the small parameter). The multigroup transport equations were thereby decoupled through first order, and this decoupling led to multigroup diffusion equations in a development that, as was emphasized,\(^1\) was limited to the case of linearly anisotropic scattering. To build on this basic idea (for the case of linearly anisotropic scattering) in the context of the development of a homogenization theory for heterogeneous fission reactors — the problem studied here
the terms corresponding to fission neutrons born in the group as a result of fissions
induced by neutrons in other groups would have to be taken as small (second order),
in addition to those corresponding to in-scattered neutrons. But this would not be
unreasonable, since at any given time most neutrons in an energy group have under-
gone one or more scatterings within the group and therefore have not been newly
born in the group via fission or in-scattering.

References

1. H. Zhang, Rizwan-uddin and J. J. Dorning, "Systematic Homogenization and
   Self-consistent Flux and Pin Power Reconstruction for Nodal Diffusion Methods.


3. E. W. Larsen, "Neutron Transport and Diffusion in Inhomogeneous Media. II,

4. H. Zhang, "Multiple-Scale Systematic Homogenization Theories for Nodal Meth-
   ods," Ph.D. Dissertation, Department of Mechanical, Aerospace and Nuclear
   Engineering, University of Virginia, Charlottesville, VA, January, 1995.

5. R. T. Chiang and J. Dorning, "A Homogenization Theory for Lattices with
   Burnup and Non-uniform Loadings" in 1980 Advances in Reactor Physics and

6. J. Dorning, "Modern Coarse-Mesh Methods — A Development of the '70s," in

7. A. Ougouag and H. Rajic, "ILLICO-HO: A Self-Consistent Higher Order Coarse-

8. R. D. Lawrence and J. J. Dorning, "A Nodal Integral Transport Theory Method
   for Multidimensional Reactor Physics and Shielding Calculations," in 1980 Ad-


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