



# An incident flux expansion transport theory method suitable for coupling to diffusion theory methods in hexagonal geometry



Robert M. Hayward, Farzad Rahnema\*, Ding kang Zhang

*Nuclear and Radiological Engineering and Medical Physics Programs, Georgia Institute of Technology, 770 State Street NW, Atlanta, GA 30332-745, USA*

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## ABSTRACT

A new hybrid stochastic–deterministic transport theory method, which is designed to couple with diffusion theory, is presented. The new method is an extension of the incident flux response expansion method, and it combines the speed of diffusion theory with the accuracy of transport theory. With ease of use in mind, the new method is derived in such a way that it can be implemented with only minimal modifications to an existing diffusion theory method. A new angular expansion, which is necessary for the diffusion theory coupling, is developed in 2D and 3D. The method is implemented in 2D hexagonal geometry, and an HTTR benchmark problem is used to test its accuracy in a standalone configuration. It is found that the new method produces excellent results (with average relative error in partial current less than 0.033%) when compared with Monte Carlo reference solutions. Furthermore, the method is fast, solving all test cases in less than 12 s.

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## 1. Introduction

The design of nuclear reactors involves frequent calculations to determine core eigenvalues and power shapes. Ideally, these calculations would be performed with the most accurate transport theory methods available, whether stochastic or deterministic. However, these most-accurate methods typically require hours, days, or even weeks of computing time to deliver results. For routine design calculations, this may not be practical, and reactor designers often compromise by using methods based on diffusion theory or low order transport, which trade accuracy for speed.

The solution of a whole-core eigenvalue problem with the current generation of diffusion theory methods typically involves a two-step procedure (Lawrence, 1986; Smith, 1986):

1. Calculate homogenized parameters (cross-sections and discontinuity factors) for each lattice cell (for example an assembly) using a detailed, transport theory calculation with specularly reflective boundary conditions.
2. Use the homogenized parameters in a nodal diffusion theory calculation to compute the whole-core solution.

For this procedure to result in accurate solutions, at least a couple of assumptions must be satisfied. The first assumption is that

the homogenized parameters (generated with zero leakage boundary conditions) are insensitive to the presence of inter-assembly leakage. In general this does not hold for configurations with core and assembly heterogeneity. The second assumption is that nodal diffusion theory provides an adequate approximation to neutron transport theory. However, diffusion theory breaks down in the presence of strong absorbers and near heterogeneous material interfaces (Stacey, 2007).

In reality, nodal diffusion theory produces results that are “good enough” when used to model the current generation of operating Light Water Reactors (LWRs). However, the limitations of the two-step homogenization–diffusion process are manifest when it is applied to prismatic gas-cooled reactors such as the (very) high temperature gas-cooled reactor (VHTR) designs. Because they are highly heterogeneous and optically thin, these reactors challenge methodologies that rely on homogenization and diffusion theory for whole-core calculations.

This work will present a fully heterogeneous transport theory method suitable for coupling to diffusion theory methods in hexagonal geometry. Because the method is based on transport theory and because it is fully heterogeneous, it requires neither of the above stated assumptions to produce accurate results. The method is designed to work alongside existing diffusion theory codes. Thus, one can use heterogeneous transport theory where diffusion theory breaks down while retaining the use of diffusion theory where it provides an adequate approximation. In this way the methodology is both fast and accurate.

\* Corresponding author.

E-mail address: [farzad@gatech.edu](mailto:farzad@gatech.edu) (F. Rahnema).

### 1.1. Methods for nodal diffusion theory in hexagonal geometry

There has been a large amount of research aimed at validating various strategies for nodal diffusion theory in hexagonal geometry (Arkuszewski, 1986; Chao and Shatilla, 1995; Cho et al., 2001; Cho and Kim, 1998; Cho and Lee, 2006; González-Pintor et al., 2009; Knight et al., 1995; Lee and Cho, 2006; Lozano et al., 2010; Tomašević and Müller, 2009; Xia and Xie, 2006; Zimin and Baturin, 2002), and most of these works demonstrate nodal diffusion theory methods with excellent agreement (less than 50 pcm error in eigenvalue and less than 1% error in assembly powers) to reference solutions. In all of these studies, however, a fine-mesh diffusion theory code is used to calculate the reference solution, and the reference solution is performed with homogenized blocks. Thus, these works mainly demonstrate that the various coarse-mesh diffusion theory methods can reproduce the solutions of fine-mesh diffusion theory methods given the same homogenized cross-sections.

In some cases, even code-to-code comparison between hexagonal diffusion theory methods produces large discrepancies. A study of steady-state VVER-1000 benchmarks—prompted by discrepancies in previous transient benchmarks—found eigenvalue differences of 470–910 pcm and assembly power differences up to 6.6% between two diffusion methods in hexagonal geometry (Ivanov et al., 2006). Because both methods used the same set of cross sections, these results are attributed to differences between the two treatments of hexagonal geometry and also to high flux gradients at the fuel-reflector boundary.

When the coupled RELAP5/PARCS code was used in a study of the VVER-1000 coolant trip benchmark, errors were found to be greatest on the core periphery and inaccurate assembly discontinuity factors (ADFs) were cited as the most likely cause (Bousbia Salah et al., 2006). While it is unfair to condemn diffusion theory solely based on a transient benchmark, these results highlight a problem shared by all diffusion methods: the difficulty of modeling the core boundary.

There has been recent work aimed at enhancing DIF3D for use on prismatic VHTR problems (Lee et al., 2007, 2006a,b). This work is notable in that it compares DRAGON/DIF3D to continuous energy MCNP. This work shows the difficulty and necessity of using surface-dependent discontinuity factors (DFs). Without surface-dependent DFs, eigenvalue errors of above 1000 pcm and maximum assembly power errors of 5–12% are reported for (7-block) mini cores with either a single rodged reflector block or a single rodged fuel block. When surface-dependent DFs are introduced, eigenvalue errors are reduced to around 600 pcm and maximum assembly power errors are reduced to 1–3%. The surface-dependent DFs are generated using two different methods, but each method involves the transport theory solution of (7 block) mini core problems. This type of computation is not practical for routine reactor design calculations. In whole core VHTR problems the eigenvalue errors can be over 600 pcm with maximum assembly power errors of 5–12% near control rods even with the use of surface-dependent DFs.

### 1.2. Methods for whole-core transport theory in hexagonal geometry

It is clear that diffusion theory alone is not sufficient to handle VHTRs with high accuracy, especially in the vicinity of control rods. Whole-core transport theory, however, can provide good results for VHTRs. Stochastic methods, such as MCNP (Brown et al., 2002), can solve the continuous energy transport equation with high geometric accuracy even for complex and irregular geometries. The disadvantage of such methods is that the results are subject to statistical uncertainty. The cost of increased precision is increased computational effort, and this tradeoff is governed by the central limit theorem. For routine reactor design calculations,

this cost is prohibitively high. For example, the 2D whole-core reference solutions in section IV of this paper were determined with MCNP5, and each required between 3 and 6 h running in parallel across 12 compute nodes (a total of 96 CPU cores).

Unlike stochastic methods, deterministic transport methods do not suffer from limited statistical precision. Deterministic transport methods are instead limited by discretization error, which can be reduced by refining the computational mesh (in space, energy, and angle) along with a corresponding increase in computational resources. One such multigroup deterministic transport method is DeCART. DeCART is notable among deterministic transport methods for its ability to simulate whole-core problems without homogenization (Cho et al., 2008). For 2D and 3D whole-core prismatic VHTR problems, DeCART's agreement with continuous energy MCNP is typically within 200–500 pcm for multiplication factor and within 4–5% for block-averaged power (Cho et al., 2007; Lee and Yang, 2011; Lee et al., 2010). Unfortunately, no timing information is provided for most of these results. However, one of the references indicates that it takes about 5 h to solve a 2D VHTR problem on a single CPU (Cho et al., 2007). In terms of computational resources, this is an improvement over stochastic methods, but this improvement comes at the price of accuracy.

For the design and analysis of prismatic gas-cooled reactors like VHTR, a method that is both fast and accurate is required. For this reason, a hybrid stochastic–deterministic transport theory called COMET (for Coarse Mesh Transport) has been extended to hexagonal geometry. COMET is based on the incident flux response expansion (Zhang and Rahnema, 2012) and was originally developed for fully-heterogeneous, whole-core transport theory in LWRs (Ilas and Rahnema, 2003; Mosher and Rahnema, 2006). The method has been since shown to work for Heavy Water Reactors (HWRs) (Zhang and Rahnema, 2012) and for prismatic gas-cooled reactors (Connolly et al., 2011, 2012; Connolly and Rahnema, 2012) as well. The COMET method has been compared with multigroup MCNP using the same 2D HTTR benchmark analyzed in section IV of this paper. COMET was shown to be accurate to within 30 pcm in eigenvalue and within 1% in pin power with calculation times on the order of minutes. While this is much faster than either Monte Carlo or fine mesh stochastic methods, it is still desirable to use methods that have on-the-fly speed such as diffusion theory, which can arrive at whole-core solutions in seconds.

### 1.3. The new method

We introduce a method that uses diffusion theory where it is valid while using a transport theory method elsewhere. The motivation is to create a coupled method that is competitive with transport theory for accuracy and competitive with diffusion theory for speed.

The goal of this work is to extend the incident flux response expansion transport theory method developed by Zhang and Rahnema (2012) so that it is suitable for coupling to a diffusion theory method in hexagonal geometry. The remainder of this paper is organized as follows. In Section 2 we present the method's underlying theory; in Section 3 we present the details of the method's implementation including a new angular expansion basis; and in Section 4, we demonstrate the method by solving 2D HTTR benchmark problems using the incident flux response expansion as a standalone method.

## 2. Theory

Broadly, we seek the solution (eigenvalue  $k$  and eigenfunction  $\psi, \varphi$ ) to the steady-state coupled transport–diffusion equations

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