International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C 2011)
Rio de Janeiro, RJ, Brazil, May 8-12, 2011, on CD-ROM, Latin American Section (LAS) / American Nuclear Society (ANS)
ISBN 978-85-63688-00-2

EXTENSION OF THE COMET METHOD TO 2-D HEXAGONAL GEOMETRY

Kevin John Connolly, Farzad Rahnema*, and Dingkang Zhang
Nuclear and Radiological Engineering Program
George W. Woodruff School
Georgia Institute of Technology
Atlanta, Ga., United States
farzad@gatech.edu

ABSTRACT

The capability of the heterogeneous coarse mesh radiation transport (COMET) method developed at Georgia Tech has been expanded. COMET is now able to treat hexagonal geometry in two dimensions, allowing reactor problems to be solved for those next-generation reactors which utilize prismatic block structure and hexagonal lattice geometry in their designs. The COMET method is used to solve whole core reactor analysis problems without resorting to homogenization or low-order transport approximations. The eigenvalue and fission density distribution of the reactor are determined iteratively using response functions. The method has previously proven accurate in solving PWR, BWR, and CANDU eigenvalue problems. In this paper, three simple test cases inspired by high temperature test reactor material cross sections and fuel block geometry are presented. These cases are given not in an attempt to model realistic nuclear power systems, but in order to test the ability of the improved method. Solutions determined by the new hexagonal version of COMET, COMET-Hex, are compared with solutions determined by MCNP5, and the results show the accuracy and efficiency of the improved COMET-Hex method in calculating the eigenvalue and fuel pin fission density in sample full-core problems. COMET-Hex determines the eigenvalues of these simple problems to an order of within 50 pcm of the reference solutions and all pin fission densities to an average error of 0.2%, and it requires fewer than three minutes to produce these results.

Key Words: Transport method, coarse mesh method, hybrid method, hexagonal geometry, reactor analysis.

1. INTRODUCTION

A new generation of nuclear reactors is planned which will come with features and capabilities distinct from the current fleet of reactors. Among these next-generation reactors is the very high temperature reactor (VHTR), which makes use of prismatic block assembly structure and utilizes hexagonal geometry in its design. It presents a challenge to current methods because of strong block and core heterogeneity and larger neutron mean free path (MFP) than currently operating water-moderated reactors. For example, the presence of control rods in graphite blocks breaks down diffusion theory and the larger MFP leads to more pronounced angular effects which are challenging to low order methods. It is desirable to have methods which are not prone to errors due to homogenization or low-order transport approximations.

* Corresponding author

The heterogeneous coarse mesh radiation transport (COMET) method [1, 2] has been demonstrated to perform whole-core reactor analysis efficiently and accurately. It relies solely on transport theory without homogenization or low-order transport approximations (e.g., diffusion theory). COMET solutions including eigenvalue and fuel pin fission density distribution have been shown to be highly accurate and efficient in current water-moderated reactors including BWR [3], PWR [2], and CANDU [4]. In this paper, the coarse mesh transport method is extended to solve two-dimensional problems with hexagonal lattice structure.

A brief overview of the method is presented in the following section. Three simple test problems are presented in the third section to test the accuracy and computational efficiency of the COMET method against Monte Carlo reference solutions. A discussion of the results and some concluding remarks are found in the fourth and fifth sections of this paper.

2. METHODS

The COMET method [2], with its basis in the incident flux response expansion method [1], determines the eigenvalue of a system and also the fission density of every fuel pin in the core. It does this by breaking up the entire system into a set of non-overlapping sub-volumes, or coarse meshes. Each coarse mesh becomes the domain of a fixed source problem, and each is coupled to the adjacent coarse meshes via the angular current at their interfaces. Solutions to these fixed-source problems, which are referred to as response functions since they are the response to a known incoming current, are pre-computed for each unique mesh. An iterative process uses the collection of response functions to determine the solution to the original problem.

2.1. Overview of COMET

In order to solve a whole-core eigenvalue problem, the COMET method divides it into a series of local fixed source problems, each of which is defined over a coarse mesh. In a prismatic gas-cooled reactor, a typical coarse mesh would be the size of a fuel block. The transport equation for a fixed-source problem within a coarse mesh is given as equation (1), in which $\vec{r}$, $\hat{\Omega}$, and E designate the position, angle, and energy of interest; ψ_i denotes the angular flux within mesh i; σ_t, σ_s, and σ_f represent the macroscopic total, scattering, and fission cross sections, respectively; an average of ν neutrons are produced per fission event from the energy spectrum χ; and the core eigenvalue is $\frac{1}{k}$:

$$\begin{aligned}\hat{\Omega}\cdot\nabla\psi_i\left(\vec{r},E,\hat{\Omega}\right)+\sigma_t\left(\vec{r},E\right)\psi_i\left(\vec{r},E,\hat{\Omega}\right)=\int_0^\infty dE'\int_{4\pi}d\hat{\Omega}'\sigma_s\left(\vec{r},E',\hat{\Omega}'\to E,\hat{\Omega}\right)\psi_i\left(\vec{r},\hat{\Omega}',E'\right)\\+\frac{1}{4\pi}\chi\left(\vec{r},E\right)\int_0^\infty dE'\int_{4\pi}d\hat{\Omega}'\frac{\nu\sigma_f\left(\vec{r},E',\hat{\Omega}'\right)}{k}\psi_i\left(\vec{r},\hat{\Omega}',E'\right)\end{aligned} \tag{1}$$

Each mesh has as a boundary condition equation (2):

$$\psi_i\left(\vec{r}_{ij},\hat{\Omega}_i,E\right)=\psi_j\left(\vec{r}_{ij},\hat{\Omega}_j,E\right) \tag{2}$$

Mesh *i* and mesh *j* meet at the surface defined by r_{ij}. With $\hat{n}_i$ being the outward normal vector from mesh i, $\hat{n}_i \cdot \hat{\Omega}_i = -\hat{n}_j \cdot \hat{\Omega}_j$. In the special case where the boundary of mesh *i* coincides with the external boundary of the core, the boundary condition of that mesh face is simply the same as that of the system. The boundary condition can also be given in terms of the angular current *J*, as shown in equation (3):

$$J_i\left(\vec{r}_{ij},\hat{\Omega}_i,E\right)=J_j\left(\vec{r}_{ij},\hat{\Omega}_j,E\right) \tag{3}$$

The remainder of this paper will use angular current to describe the boundary conditions of the coarse meshes. For the problems illustrated in this paper, the external boundary of each core will be taken as no incoming current. This is not a restriction on the method in general.

A response function generating module computes the outgoing current from each face *f'* and the fission density within each pin of a mesh as a response to a given incoming current from face *f*. To model this, COMET treats the angular current distribution as a combination of the shifted Legendre polynomials which have as their domain the position *u* along the mesh face, the azimuthal angle φ and cosine μ of the polar angle of the neutron direction with respect to the mesh face, as shown in equations (4) and (5). Any other functions orthogonal over the angular half-space could have alternately been used. The multigroup method is used to treat the energy dependence of the current.

$$J_f^{in}=\delta\left(E-E_g\right)P_m^{[0,U]}(u)P_n^{[-1,1]}(\mu)P_p^{[0,\pi]}(\varphi) \tag{4}$$

The outgoing angular current from each face can be determined to a high degree of accuracy even when the series of Legendre polynomials is truncated at a low order, such as shown in equation (5):

$$J_{f'}^{out}\approx\sum_{g=1}^{G}\sum_{m=0}^{M}\sum_{n=0}^{N}\sum_{p=0}^{P}c_{gmnp}\delta\left(E-E_g\right)P_m^{[0,U]}(u)P_n^{[-1,1]}(\mu)P_p^{[0,\pi]}(\varphi) \tag{5}$$

This method may be used to find other quantities of interest, such as reaction rates within a region of the coarse mesh. For example, fission reaction rates are tallied in individual pins. Results are calculated for all values of *f* and *g* present in the problem, for all *m*, *n*, and *p* desired in calculating in equation (4).

An iterative sweeping procedure is used to find the solution of the problem. One iterative loop is used to determine the eigenvalue of the system starting with an initial guess. A series of inner iterations is conducted which sweeps across the volume of the system, using the concept of linear superposition to determine the outgoing current from every coarse mesh based on the incoming current from the previous iteration. Once the values for the current at all mesh boundaries converge to a desired criterion, the system eigenvalue is re-calculated using the neutron balance method and the process repeats until the eigenvalue converges.

2.2. New Capabilities of COMET-Hex

The COMET method uses Monte Carlo methods to solve the series of fixed-source transport problems [2]. A modified version of MCNP5 [5] is used to transport the source particles given an angular current distribution such as the one in equation (4). A separate fixed-source calculation is conducted for each different combination of the values of f, g, m, n, and p for each unique coarse mesh, and at differing values of the core eigenvalue for coarse meshes containing multiplying media. The outgoing current is tallied at each face and output in terms of the desired expansion order of Legendre polynomials. The coefficients c of the solutions from equation (5) are tabulated and stored in a database.

Because COMET-Hex defines the angular current in reference to each mesh face, and because the geometry system used in MCNP5 makes use of Cartesian coordinates, a series of coordinate transformations must be introduced into the source and tally definitions to operate in hexagonal geometry. The response function generator for COMET-Hex samples source particles randomly from distributions over u, φ, and μ. Not all of these coordinates correspond to coordinates in the Cartesian MCNP reference system, which defines position in the x, y, and z directions, and angle in Ω_x, Ω_y, and Ω_z components. Each COMET-Hex coordinate, once selected, must be transformed into the MCNP reference system in order to perform transport calculations. When a particle exits the mesh, its position and angle must be transformed from MCNP's coordinate system back into COMET-Hex's reference system, that of the mesh face.

An iterative sweeping process is used to determine the angular current at the mesh interfaces and the eigenvalue of the core. Since at present, COMET-Hex only treats full hexagonal meshes, the sweeping process must be conducted over the whole core even if it exhibits some form of symmetry. Furthermore, a core with one-sixth symmetry cannot be swept in such a way to preserve symmetry in all six directions. However, due to the pre-computation of the response function library and the choice of convergence criteria, the mesh sweeping order and direction are not believed to have an effect on the accuracy of the final calculated solution. Future work includes an investigation of the sweeping procedure to determine its effect, if any, on the problem solution.

COMET-Hex is implemented in Fortran 95.

3. TEST PROBLEMS

Because COMET-Hex is under development, it is desirable to test its performance with very simple problems. The problems illustrated here are not intended to portray realistic reactor designs, but merely to serve as test problems for methods development and error diagnostics. They are presented only to challenge the code's handling of sharp flux gradients, material boundaries, regions of high neutron leakage and absorption, and asymmetric systems. These test problems use the block structure and six-group cross section data from a benchmark problem [6] based on the high temperature test reactor. Each core consists of three rings of prismatic blocks around a center block. The boundary of the system is corrugated as COMET-Hex handles only full blocks at present. A boundary condition of no re-entrant particles is specified.

Three unique types of blocks are present in the core. The first is a fuel block, which is modeled as a hexagonal prismatic block of graphite with 33 fuel pins and 3 absorber pins. The fuel is treated as a pin consisting of a homogeneous mixture of graphite and a 4.3% enriched uranium oxide fuel compact, neglecting the heterogeneity due to the coated fuel particles in a graphite matrix. The absorber is a combination of boron carbide and carbon. In two of the test problems, control blocks are present which are modeled as graphite blocks with a single boron carbide control rod in the center. Reflector blocks are also present which consist solely of graphite. The three types of block geometry used are shown in Fig. 1.

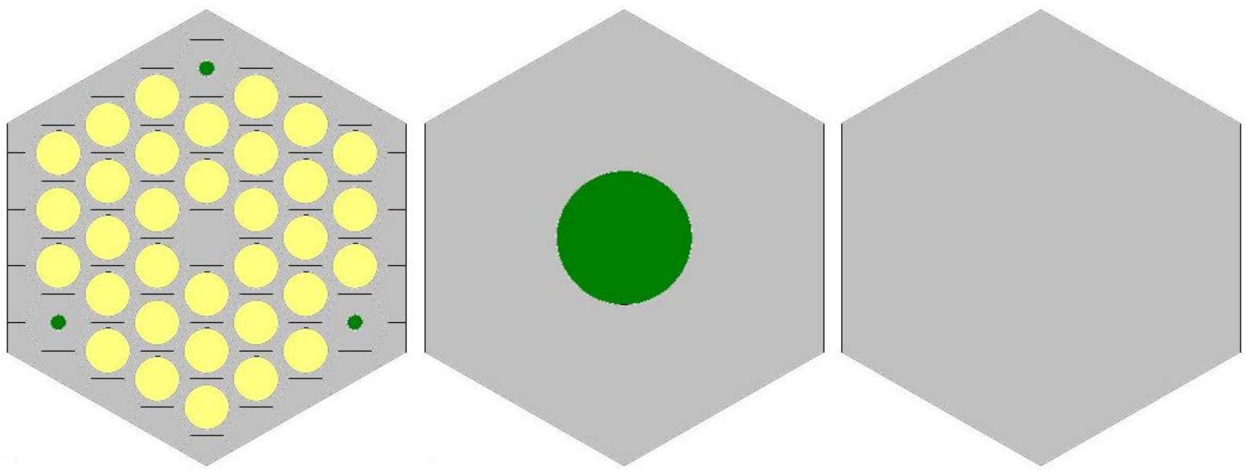

Figure 1. Fuel, control, and reflector blocks

As the first preliminary test, the simplest problem is presented. Let the first problem consist entirely of fuel blocks, as depicted in Fig. 2. This test is intended to challenge the performance of COMET-Hex in a system with large flux gradients and a large amount of leakage.

MCNP5 was used to acquire a reference solution. Five hundred million active particle histories were sampled for tallying after 62.5 million particle histories were skipped to converge the fission source. The system eigenvalue was found to be 0.84309 +/- 0.00003. The average statistical uncertainty in the pin fission densities was 0.067%, with the maximum pin fission density uncertainty at 0.19% for the six pins at the outermost corners of the core. All calculations presented in this paper were performed using 2 GHz processors with 16 GB of memory per eight-processor node. This calculation required 60.5 days of total computing time using 64 processors running in parallel.

As the first problem is quite simple, a second problem is now presented. The aim of the test is to introduce differing types of coarse meshes so as to challenge COMET's performance in heterogeneous systems. This problem places a control block at the center of the reactor, and surrounds the core with reflectors. The core geometry is illustrated in Fig. 3. A reference solution was calculated in MCNP5 in which 500 million particle histories were sampled for tallying after skipping 62.5 million particle histories. The eigenvalue of the core was calculated to be 0.82156 +/- 0.00003. All pin fission densities were calculated to a statistical uncertainty of between 0.03% and 0.05%. This calculation required 63.7 days of computing time using 32 processors running in parallel.

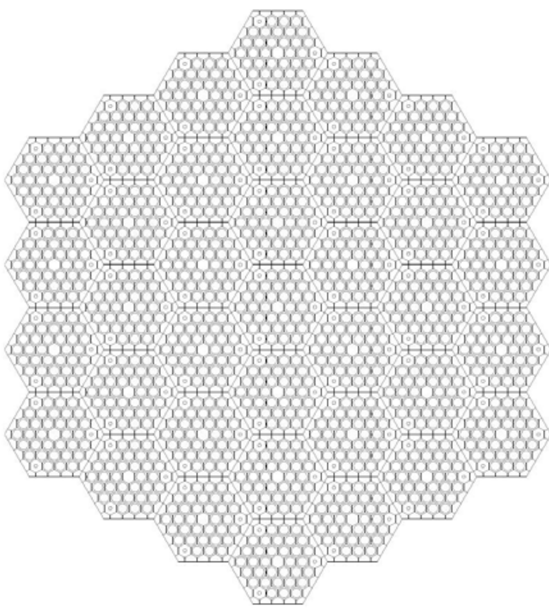

Figure 2. Test core #1

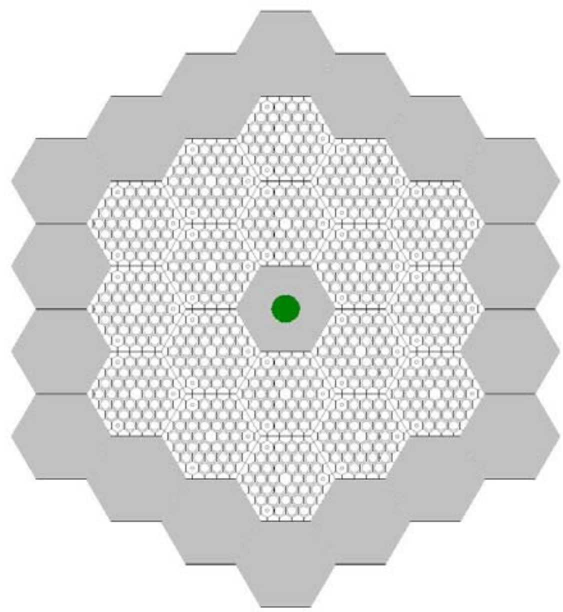

Figure 3. Test core #2

Now, in order to present a greater challenge to the capabilities of the COMET method, a third and final problem is presented. This test case includes 27 fuel blocks, 4 reflector blocks, and 6 control blocks arranged as shown in Fig. 4. The power profile in the region surrounded by control blocks will be of special interest; low errors will demonstrate COMET's accuracy even near absorbers. Furthermore, the core is asymmetric in order to illustrate that the hexagonal coarse mesh method does not require symmetric problems to produce accurate solutions. The reference solution was calculated in MCNP as in the previous cases, skipping 62.5 million particle histories before running 500 million particle histories for tallying. This core eigenvalue was found to be 0.70840 +/- 0.00003. The average statistical uncertainty of the pin fission density tallies was 0.069%, with a maximum pin fission density uncertainty of 0.30%. All uncertainties over 0.2% were found in the fuel block on the outermost ring, in the corner, between the edge of the core and the control assemblies. This calculation took 54.2 days of computing time on 16 processors running in parallel.

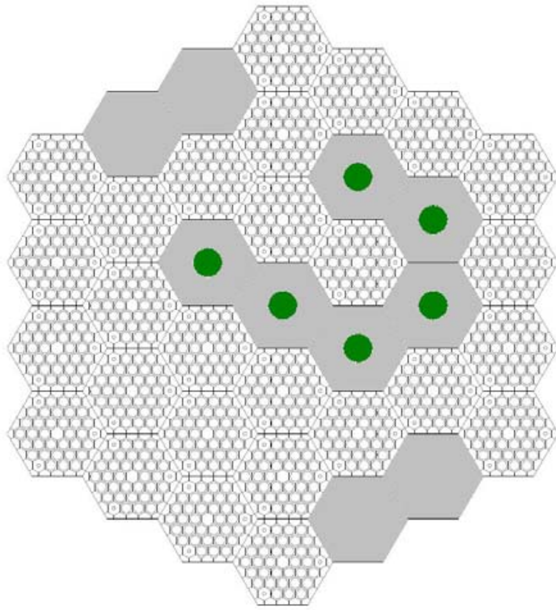

Figure 4. Test core #3

4. RESULTS

In order to solve these problems, the response function generator performed a total of 13,500 response function calculations, each requiring 10 million particle histories. A typical response function calculation for a fuel block required 12.5 minutes of computing time on a single processor; a typical calculation for a block without fuel required 2.75 minutes. The entire response function library was calculated in approximately 30 hours using 64 processors, roughly 80 days of total computing time. The collection of response functions was compiled in a database requiring 24.00 minutes on a single processor to complete. This database may be used for any reactor physics calculation with these assemblies and a core eigenvalue between 0.67 and 0.87.

COMET results are presented in Tables I-III. Included in each table are the expansion orders for which the calculation was carried out in space, cosine of the polar angle, and azimuthal angle. That is, (M, N, P) in the first row of the table represents the order at which summations over m, n, and p from equation (5) are truncated. High order cross terms in the angular component of the flux were eliminated to conserve expansion order; that is, moments of the flux in which $(N+P) > 4$ were neglected.

The relative difference between the reference solution and the COMET solution for the eigenvalue is presented in the table for each test case and given in per cent mille. The four rows which follow show the differences in the calculation of the pin fission densities; they include the average relative error between the COMET solution and the reference solution, the root mean squared error, the mean relative error, and the maximum relative error. Pin fission density results are given as per cent relative errors. For the sake of the results presented in this paper, the definition used for the relative error in some quantity q will be as given in equation (6):

$$RE_q = \frac{q_{COMET} - q_{MCNP5}}{q_{MCNP5}} \tag{6}$$

The final value presented in each table is the computing time required to complete the calculation, given in seconds. Computation was conducted on a single processor.

All solutions utilized the same convergence criteria. Inner iterations on the current used a convergence ratio of 5×10^{-5}. As a safety check for inner iteration convergence, pin fission densities converged to 10^{-4}. Outer iterations on the eigenvalue used a convergence criterion of 5×10^{-5}.

The results for test core #1 are presented in Table I. In each of the four different expansion order calculations, COMET determined the eigenvalue to an uncertainty of between 7.5 and 8 pcm. The average relative uncertainty in the pin fission densities was 0.08%, with a range from 0.05% to 0.21%. In each calculation, the only six pins in the reactor with uncertainties in the fission density of over 0.2% were the pins at the corners of the hexagonal-shaped core where flux was lowest.

Table I. Test core #1 results

	(2,2,2)	(4,2,2)	(2,4,4)	(4,4,4)
k (pcm)	99	110	40	50
AVG (%)	0.240	0.226	0.229	0.227
RMS (%)	0.394	0.299	0.298	0.288
MRE (%)	0.173	0.168	0.171	0.173
MAX (%)	1.686	1.518	1.518	1.350
time (s)	32.7	75.6	59.7	162.3

Core #1 includes 1221 fuel pins within the region. In the (4,4,4) case, 14 pins had relative errors of greater than 0.75%, and 5 of these pins had relative errors greater than 1.0%. All of these pins were found in the outermost ring of the core, where flux and fission density levels are lowest, and 13 of the 14 had fission density values of below 0.2.

The results for test core #2 are presented in Table II. In all four test cases, COMET solved the eigenvalue problem within an uncertainty of 9 pcm. Relative uncertainties for pin fission densities were between 0.053% and 0.062% for all cases. In the (2,4,4) and (4,4,4) cases, 8 pins out of the 594 in the core had errors greater than 0.5%. All of these fuel pins were found in the outermost rings of fuel blocks at the corners.

The lower errors in the pin fission density calculations in core #2 when compared with core #1 may be a result of the flatter flux profile in the second core. Core #1 is a bare reactor with a peaking factor of 2.347, and the pin with the lowest fission density in the first core has a value of only 0.059. In contrast, core #2 is surrounded by reflector blocks and has a control block in the center of the core. The fission densities of pins within the core range from 0.726 to 1.363.

Table II. Test core #2 results

	(2,2,2)	(4,2,2)	(2,4,4)	(4,4,4)
k (pcm)	106	112	52	59
AVG (%)	0.189	0.186	0.188	0.188
RMS (%)	0.229	0.226	0.227	0.228
MRE (%)	0.182	0.179	0.181	0.181
MAX (%)	0.695	0.682	0.591	0.603
time (s)	29.6	57.0	57.3	142.9

The results for the final test core are given in Table III. COMET's uncertainty in the eigenvalue calculations was between 8.3 and 8.6 pcm in all four calculations. COMET calculated the pin fission densities to an average uncertainty of 0.081% in the (2,2,2) calculation and 0.083% in the (4,4,4) calculation. The maximum uncertainty in COMET's determination of the fission density in the (4,4,4) case was 0.221%; 7 pins had uncertainties in the fission density calculation of greater than 0.2%, all of which were on the corners of the reactor where flux is lowest. The uncertainty in the lower order calculations was slightly lower, but by less than 0.002% on average and by less than 0.005% in the highest uncertainty pins.

The range of power levels within core #3 was the highest of the three test cores. The peaking factor was 2.451, and the lowest pin fission density in the core was only 0.022.

Table III. Test core #3 results

	(2,2,2)	(4,2,2)	(2,4,4)	(4,4,4)
k (pcm)	82	90	18	27
AVG (%)	0.220	0.206	0.190	0.184
RMS (%)	0.296	0.271	0.250	0.239
MRE (%)	0.164	0.162	0.144	0.142
MAX (%)	1.244	1.158	0.933	0.933
time (s)	64.8	151.3	172.7	451.3

Of special interest in core #3 was the fuel block surrounded on five sides by control blocks. For the (4,4,4) calculation, the average relative error in the pin fission densities in this block was 0.122%, with a maximum error of 0.316%. The root mean squared error of the pins within this block was 0.147%. These low errors show that COMET calculates accurate results even in regions near strong absorbers.

Core #3 contains 891 fuel pins. Of those, only 5 pins were found to have relative fission density errors greater than 0.75% between the reference solution and the (4,4,4) COMET calculation. All of those pins were found in the outermost ring of the core, and the fission density levels of those pins ranged from 0.056 to 0.258 times the core average.

It can be seen in all three calculations that in these graphite-moderated systems, expanding the angular component of the flux from second-order to fourth-order leads to a reduction in the eigenvalue calculation by a factor of two, while expansion of the spatial component of the flux from second order to fourth order has no statistically significant effect on the eigenvalue calculation at all. In no case did the error in the eigenvalue change by greater than the convergence criteria plus σ or any of the errors in the pin fission density change by greater than the convergence criteria plus 2σ when the expansion order used was expanded from second order to fourth in the spatial variable. This is likely due to the fact that these graphite blocks have a higher neutron mean free path and a lower optical thickness. Variations in the flux due to pin-level heterogeneity will therefore be minor. It may be concluded that expansion of the spatial component of the current is unnecessary past a second-order expansion; if response function calculations were not conducted for expansion orders in space greater than 2, 40% fewer response function calculations would be performed.

The efficiency of the COMET-Hex method can easily be seen. For each different core, MCNP reference solutions took many days of computing time to calculate. In contrast, COMET-Hex required a one-time computation of a response function library which took less computing time to complete than two full-core reference solutions. After that pre-computation was complete, COMET-Hex was able to solve whole-core test problems exhibiting a range of eigenvalues and pin fission density levels in only a few minutes.

5. CONCLUSIONS

Preliminary tests and results for the hexagonal coarse mesh transport method have been presented. Solutions are reached in a few minutes and have been shown to agree very well with calculated reference solutions to an order of 50 pcm in eigenvalue and 0.2% in pin power. Future work will include using COMET-Hex to solve benchmark problems based on realistic reactor geometry. It is expected that this method will yield results of realistic reactor problems just as accurately and quickly as for the preliminary tests presented here.

The method and solution processes presented in this paper do not utilize any acceleration techniques, and simplifications are not made to take advantage of symmetry within the meshes. Including a method within the response function generator to treat symmetry within coarse meshes could decrease the time necessary for this module by a factor of three or even six. Acceleration techniques used in the Cartesian version of COMET [2] have been shown to reduce the time required to solve a full-core problem; it is anticipated that similar tactics could be used to converge COMET-Hex to the solution more quickly.

Future work will include an extension of this method to three dimensions. It is anticipated that a three-dimensional version of COMET-Hex will prove a useful tool for the accurate and fast analysis of whole prismatic block reactor cores.

ACKNOWLEDGEMENTS

The first author's work was supported under a Department of Energy Nuclear Energy University Program (NEUP) Graduate Fellowship. The other authors' effort was supported by NEUP Award Number DE-AC07-O5ID14517. Any opinions, findings, conclusions, or recommendations expressed in this publication are those of the authors and do not necessarily reflect the views of the Department of Energy Office of Nuclear Energy.

REFERENCES

1. S. W. Mosher and F. Rahnema, "The Incident Flux Response Expansion Method for Heterogeneous Coarse Mesh Transport Problems," *Transport Theory and Statistical Physics*, **35**, pp. 55-86 (2006).
2. B. Forget and F. Rahnema, "COMET Solutions to the 3-D C5G7 MOX Benchmark Problem," *Progress in Nuclear Energy*, **48**, pp. 467-75 (2006).
3. B. Forget and F. Rahnema, "COMET Solution in a Highly Heterogeneous Boiling Water Reactor Benchmark Problem," *Transactions of the American Nuclear Society*, **95**, pp. 709-12 (2006).
4. B. Forget and F. Rahnema, "COMET Solutions to Whole Core CANDU-6 Benchmark Problem," *PHYSOR-2006: Advances in Nuclear Analysis and Simulation*, American Nuclear Society's Topical Meeting on Reactor Physics, Vancouver, Canada, September 10-14 (2006).
5. X-5 Monte Carlo Team, "MCNP—A General Monte Carlo N-Particle Transport Code, Version 5," Los Alamos National Laboratory (2005).
6. Z. Zhang, F. Rahnema, J. M. Pounders, D. Zhang, and A. Ougouag, "A Simplified 2D HTTR Benchmark Problem," *International Conference on Mathematics, Computational Methods & Reactor Physics (M&C 2009)*, Saratoga Springs, New York, May 3-7, 2009, on CD-ROM, American Nuclear Society, LaGrange Park, Ill. (2009).