

## Whole-Core Transport Solutions to A Stylized CANDU-6 Core Problem

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### Abstract

A stylized CANDU half core with adjuster rods was used to test the accuracy and efficiency of the coarse mesh transport (COMET) code. The benchmark problem consists of 2280 fuel bundles in 190 fuel channels with 8 different burnups. The model includes a total of 21 adjuster rods of 1 type perpendicular to the fuel channels and located on three axial locations. A modified version of the MCNP code was used to generate the response function library in the pre-computation phase, and the COMET was used to compute the global eigenvalue and bundle/pin power distribution. In these calculations, a set of tensor products of orthogonal polynomials were used to expand the neutron angular phase space distributions on the interfaces between coarse meshes. The COMET calculations were compared with the MCNP reference solutions. The comparison showed both the global eigenvalue and bundle/pin power distributions predicated by COMET agree very well with the MCNP reference solution if the orders of expansion in the two spatial variables and the polar and azimuth angles are 4, 4, 2 and 2. These comparisons indicate that COMET can achieve accuracy comparable to Monte Carlo methods while maintaining computational efficiency significantly (orders of magnitude) faster than that of MCNP.

### 1. Introduction

A coarse mesh radiation transport (COMET) method [1] has been developed for neutronics analyses of light and heavy water reactors. The method consists of local transport calculations of incident flux response expansion functions, a two-level sweeping technique to determine the global eigenvalue, and construction of the global fuel pin-power distribution. A method within the stochastic (Monte Carlo) framework pre-calculates local response expansion coefficients for each unique assembly/bundle as a library for COMET. The use of the Monte Carlo method for computation of the local expansion coefficients allows the material heterogeneity and geometric complexity of fuel bundles and other material in the core (e.g., adjuster rods) to be explicitly modeled without using homogenized cross sections. COMET has been benchmarked in simplified BWR and PWR configurations [2-4] at hot operating conditions. The results have shown that COMET is highly accurate and efficient as compared to whole core Monte Carlo results.

The primary objective of this paper is to test the accuracy and computational performance of the COMET code for a stylized CANDU problem with adjuster rods at the hot operating (cooled) and voided conditions. The paper is organized as follows. The COMET method is briefly introduced in section 2. Section 3 describes the CANDU half core benchmark problem. The COMET calculations are presented in section 4. The conclusion is drawn in section 5.

## 2. COMET method

The COMET method divides a global spatial domain (e.g., a reactor core) into a number of non-overlapping coarse meshes and uses a pre-computed library of local (single mesh) response functions to solve for the whole core solution, based on a two-level deterministic iteration method. In the inner iterations, the pre-computed response function library is repeatedly used to converge on the outgoing fluxes from each coarse mesh. In the outer iterations, the particle balance equation is used to converge on the core eigenvalue. These response functions are solutions to a set of fixed source transport problems for each unique coarse mesh in vacuum with a unit incoming surface source with the phase space distribution specified by a complete set of orthogonal functions (such as Legendre polynomials). It has been shown that this method achieves very high accuracy and computational efficiency as long as the actual particle phase distribution on the coarse mesh boundary can be sufficiently represented by a relatively low-order expansion. A detailed description of the COMET method can be found in references [1].

## 3. CANDU-6 half core benchmark

A 3D stylized CANDU core problem developed in reference [5] is used to test COMET. The core geometry, the bundle-averaged burnup distribution, void states, adjuster rod positions are briefly described in the following subsections.

### 3.1 Geometric configuration and burnup distribution

The x-y (radial) and x-z (axial) planes of the half core model are shown in Figures 1 and 2, respectively. The problem consists of 190 (radial)  $\times$  12 (axial) fuel bundles, which are exact representations of CANDU-6 NU (Natural Uranium) 37-fuel-element bundles shown in Figure 3. The dimension of the fuel bundles is 28.575 cm  $\times$  28.575 cm  $\times$  49.53 cm. The peripheral fuel channels are surrounded by a corrugated reflector with a thickness of approximately 60 cm in the radial direction (see Fig. 1). A specular reflective boundary condition is imposed on the mid-plane surface, and a vacuum boundary is assumed on all other external surfaces.

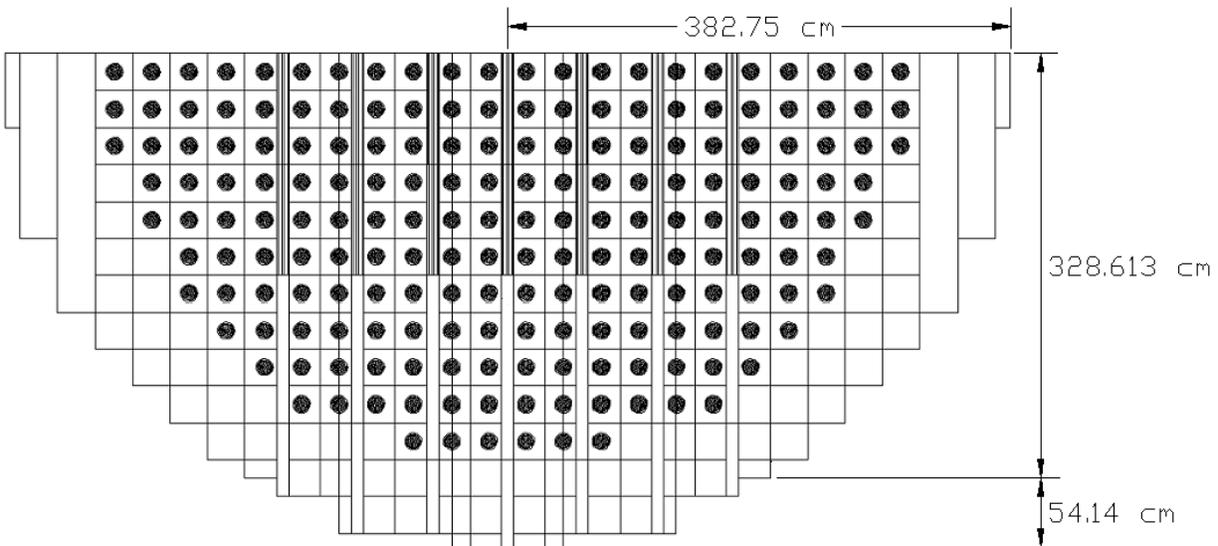


Figure 1 x-y plane (radial Slice) of the CANDU half core  
 (Showing adjuster rods in red)

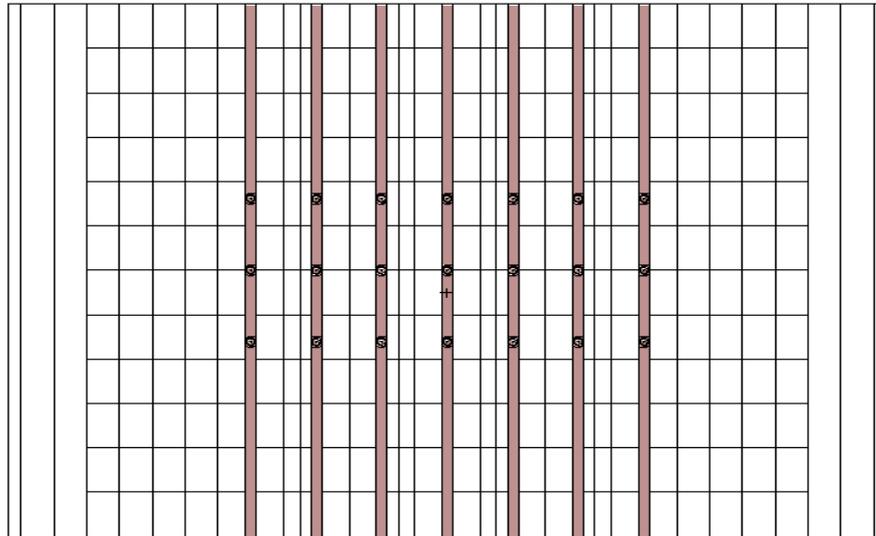


Figure 2 x-z plane of the CANDU half core

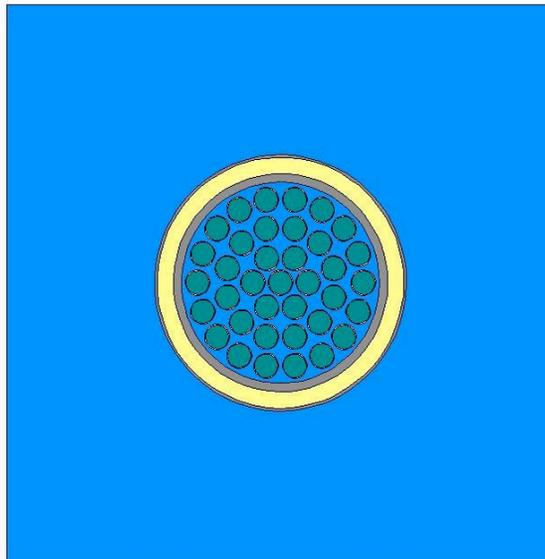


Figure 3 CANDU-6 lattice representation

The above problem is a stylized core with a simplified burnup distribution. The burnup of the fuel bundles in the core corresponds to one of the following eight discrete burnup points: 32.69, 78.38, 342.37, 818.87, 1638.73, 3608.15, 6381.44 and 8721.49 MWd/tU. The detailed burnup distribution in the core can be found in reference 6. The core is assumed to be symmetric about the horizontal radial mid-plane. As a result, only half of the core is modeled with specular reflective boundary condition on the plane of symmetry.

### 3.2 Void states

The two core configurations examined correspond to the cooled and fully voided. The cooled state corresponds to the coolant and moderator at nominal hot operating condition. The fully voided state corresponds to a reduction in the coolant density to  $0.001 \text{ g/cm}^3$  in all channels.

### 3.3 Adjuster rods

Adjuster rods are preset in all three core configurations. As shown in Fig. 2 for the half-core geometry, the adjuster rods are parallel with the vertical direction and extend down from the mid-plane a distance of two or six bundle widths (57.15 or 171.45 cm) at seven locations in the horizontal direction. This array of adjuster rods exists on three axial planes corresponding to  $z = 217.49, 297.179$  and  $377.179$ , where  $z = 0$  is the exterior boundary of axial plane 1.

## 4. Numerical results

The 2-group material region macroscopic cross sections obtained from HELIOS [6] were used to perform the COMET and MCNP [7] calculations for the cooled and the two voided cases in the half core problem.

### 4.1 Monte Carlo calculations

The fission source for each configuration was converged by running 4500 inactive cycles with 200,000 particles per cycle. For the first case, an initial source guess was created by specifying source particle locations within each fuel pin at each of the 12 axial levels using MCNP's ksrc card. Since every case has the same geometry, a converged source from a previous run was used as the initial guess to accelerate source convergence of the other cases.

Source convergence indicators included in MCNP were examined to ensure that the fission source for each case was well converged. These included verifying that cycle estimates of keff appear normally distributed, that there are no gross trends in the keff estimate and the Shannon entropy of the source is sufficiently constant.

Upon converging the fission source, an additional 3500 active cycles were executed with 200,000 particles per cycle (700 million particles total) to generate the reference solution including the core eigenvalue, the bundle fission density distribution and pin fission densities in selected bundles in the core. Pin fission densities were tallied for x-z fuel planes 13 and 21 of Figure 1.

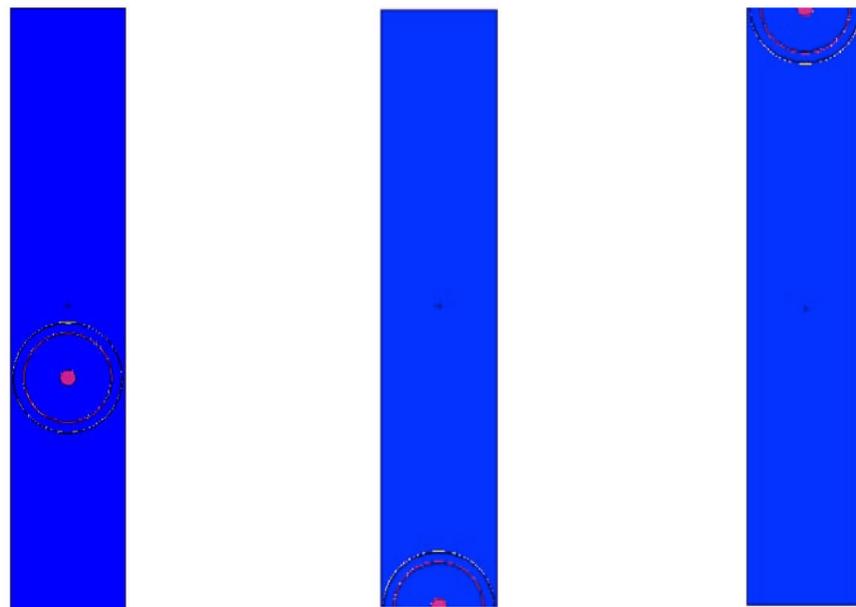
### 4.2 COMET calculations

Despite the fact the benchmark problem can be modeled in a half-core with a reflective boundary, a whole-core calculation was performed in order to demonstrate the capabilities and high efficiency of COMET. Sixty nine unique coarse meshes were used to model the cooled and voided configurations in COMET as described below:

- 24 coarse fuel meshes with the coolant at hot operating condition
- 24 coarse fuel meshes with the coolant voided
- 12 coarse meshes containing an adjuster rod and guide tube with different radii at different positions
- 9 coarse meshes of water with different sizes

Two fuel mesh sizes were used by COMET, namely,  $28.575 \text{ cm} \times 28.575 \text{ cm}$  and  $23.775 \text{ cm} \times 28.575 \text{ cm}$  in the radial direction and  $49.53 \text{ cm}$  in the z-direction. The four fuel rings in each bundle were modeled exactly the same as in MCNP, with each ring using a different set of fuel macroscopic cross sections taken from reference [5].

There are a total of 21 adjuster rods inserted in the benchmark problems. The adjuster rods were modeled in COMET using coarse meshes of  $9.6 \text{ cm} \times 28.575 \text{ cm} \times 49.53 \text{ cm}$ . There are six different rod dimensions and four different rod positions. This led to a total of 12 controlled meshes in the COMET model. Coarse meshes with three adjuster rod positions are shown in Figure 4. It should be noted that 16 of the controlled meshes contain only half of an adjuster rod (i.e., the rod cut in half), parallel to the direction of the guide tube as seen in Fig. 4b. This mesh is necessary for modeling the adjuster rods in the center plane of the core.



(a)  $z=19.059 \text{ cm}$

(b)  $z=0 \text{ cm}$

(c)  $z=49.53$

Figure 4 Adjuster rod coarse mesh with varying position in (x-z) view

In addition, 9 different moderator/reflector blocks with different dimensions were modeled. These blocks were used to match local geometry. It should be pointed out that the reactor core external boundary was approximated in both MCNP and COMET by using rectangular meshes as shown in Figure 1. The COMET boundary condition was made consistent with the MCNP input model. In particular, the boundary condition corresponded to assuming neutrons escaping the external boundary do not return. This is equivalent to assuming the reflector is surrounded by an infinite absorber.

The configuration of the COMET model is the same as the half-core MCNP model except for the following simplification. This simplification is made in a few peripheral reflector meshes. In particular, in some peripheral reflector meshes the following approximations are made: (1) some meshes are either replaced with an infinite absorber (the dark region in Figure 5 or (2) are extended (the grey region in Figure 5 to match the size of the neighboring mesh). It should be pointed out that COMET has the capability to model the exact geometry if a finer mesh moderator is used. This was not attempted in order to reduce the total number of unique meshes needed to model the core.

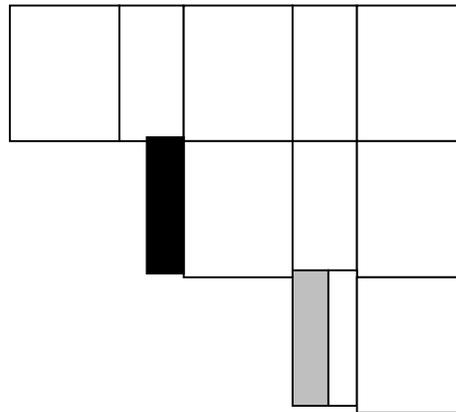


Figure 5 Simplification in COMET mesh grid

For the COMET calculations, a modified version of the MCNP code was used to generate response functions for each unique coarse mesh. For each response function (RF) calculation, 30 million histories were followed in 20 minutes on a single CPU. The uncertainty of the 0<sup>th</sup> moment of response functions were less than 0.2%. It should be pointed out that the response functions for all unique coarse meshes were generated with the maximum order of (4, 4, 2, 2) in the pre-computation phase. Note that one of the advantages of the COMET method is that once the response function library is pre-computed, criticality calculation can be performed for an arbitrary combination of the unique coarse meshes (e.g., different burnup and coolant density distributions without or with some or all adjuster rods fully or partially inserted). Using this library, COMET calculations were performed. The comparison of the core eigenvalue for the three void states is found in Table 1.

Table 1 Eigenvalue Results and the uncertainties

	MCNP		COMET		Difference (pcm)
	Eigenvalue	Uncertainty	Eigenvalue	Uncertainty	
Cooled	0.99582	0.00002	0.99633	0.00002	51
Voided	1.01166	0.00002	1.01203	0.00002	37
Voided CVR [pcm]	1584	3	1570	3	14

where the coolant void reactivity (CVR) is calculated by

$$CVR = \frac{1}{k_{cooled}} - \frac{1}{k_{voided}} \quad (1)$$

As shown in Tables 1, the core eigenvalue predicted by COMET agrees very well with that of MCNP for both cases with a difference of about 50 pcm. The coolant void reactivity computed by the two methods is also in excellent agreement. The COMET bundle averaged fission density relative differences are summarized in Table 3 for the cooled and voided cases, respectively. Note that the bundle-averaged fission density distribution is normalized to the total number of bundles in the core (2280).

Table 2 Comparison of CPU Times

are performed on a 22-

Void State	MCNP*	COMET**
Cooled	32.1	1.6
Voided	32.8	1.5

\*The MCNP calculations  
CPU cluster

\*\*The COMET calculation are performed on a single CPU

Table 3 Relative difference of bundle fission rates predicted by COMET and MCNP

Void State	Cooled	Voided
Bundle AVG (%)	0.96	0.94
Bundle RMS (%)	1.19	1.09
Bundle MRE (%)	0.91	0.90
Bundle MAX (%)	3.6	3.5

\*RE: Relative Error

AVG: Average relative difference

$avg\ RE = \frac{\sum |e_n|}{N}$ , where N is the number of fuel pins and  $e_n$  is the calculated per cent error

for the  $n$ th pin fission density,  $p_n$ .

RMS: Root Mean Square difference  $RMS = \sqrt{\frac{\sum e_n^2}{N}}$

MRE: Mean Relative difference  $MRE = \frac{\sum |e_n| \cdot p_n}{N \cdot p_{avg}}$

It can be seen that the bundle fission density for all the cooled state agree well with the MCNP results. Only 8 fuel bundles have a relative error of more than 3%. These relatively larger errors occur in the peripheral fuel regions next to the reflector blocks. This is a direct result of the simplification described above. Note that this error occurs in bundles with a low power.

A summary of the relative difference in the bundle-normalized fuel pin fission density distribution in the entire core is illustrated in Table 4. For both the cases, the difference distribution is about 0.5% on average with a maximum in the 3% to 4% range. Note that the larger differences occur in some of the peripheral bundles near the reflector meshes in which the simplification is made. It should be noted that the average and maximum uncertainties in pin fission density predicted by MCNP are about 0.53% and 1.2% and therefore the COMET agreement with MCNP is within the MCNP uncertainties in the pin fission density.

Table 4 Relative difference of pin fission rates predicted by COMET and MCNP

Void State	Cooled	Voided
Pin AVG (%)	0.45	0.48

Pin RMS (%)	0.58	0.63
Pin MRE (%)	0.45	0.48
Pin MAX (%)	3.61	3.70

## 5. Conclusion

The computational efficiency and accuracy of the coarse mesh transport method COMET was assessed for neutronics calculations in a stylized CANDU core benchmark problem with adjuster rods present in cooled and fully-voided states. The core consisted of 2280 fuel bundles in 190 fuel channels. A highly stylized burnup distribution consisting 8 different values was assumed in the core. The model included a total of 21 adjuster rods of one types at three axial locations.

The COMET model used a very coarse-mesh grid. Each mesh was one-bundle long (49.53 cm) in the axial direction. Comparisons to the MCNP reference solutions for the problem have shown that a 4<sup>th</sup> order expansion in the spatial variables and 2<sup>nd</sup> order expansion in the two angular variables are sufficient to represent the actual neutron particle distributions within the reactor core in the presence of strong heterogeneities and adjuster rods. These comparisons have also confirmed that the coarse mesh method can achieve accuracy close to Monte Carlo, while achieving a significantly faster computational efficiency (about 3 orders of magnitude).

Future work will include benchmarking COMET for a full core model with a realistic burnup distribution and including all adjuster types. The COMET method will be extended to handle cylindrical external boundary without any approximation.

## 6. Acknowledgement

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## 7. References

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