3D Heterogeneous Transport Calculations of CANDU Fuel with EVENT/HELIOS

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ABSTRACT

The applicability of the EVENT/HELIOS package to CANDU lattice cell analysis is studied in this paper. A 45-group cross section library is generated using the lattice depletion transport code HELIOS. This library is then used with the 3-D transport code EVENT to compute the pin fission densities and the multiplication constants for six configurations typical of a CANDU cell. The results are compared to those from MCNP with the same multigroup library. Differences of 70-150 pcm in multiplication constant and 0.08-0.95% in pin fission density are found for these cases. It is expected that refining the EVENT calculations can reduce these differences. This gives confidence in applying EVENT to transient analyses at the fuel pin level in a selected part of a CANDU core such as the limiting bundle during a loss of coolant accident (LOCA).

INTRODUCTION

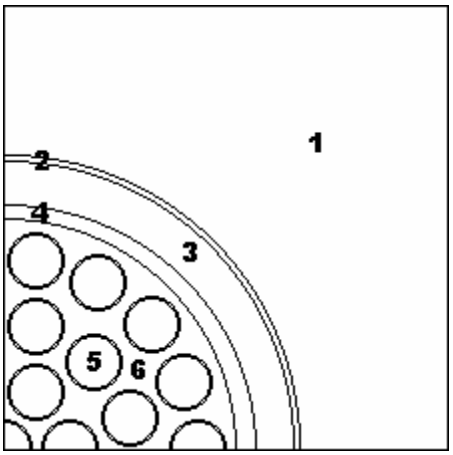
In this paper we investigate the applicability and efficiency of the deterministic transport theory code EVENT (ref. 1) for analyses of CANDU lattice cell. This is done by benchmarking the code against the Monte Carlo code MCNP (ref. 2) using 45-group cross section libraries generated by the lattice depletion code HELIOS (ref. 3). The EVENT code solves the multigroup even-parity form of the steady-state as well as the time-dependent transport equation in arbitrary geometry. It uses a finite element spatial representation and a spherical harmonics angular representation for the neutron flux. The benchmark calculations were performed at two coolant conditions (hot operating, HOC, $\rho_{HOC} = 0.80623$ g/cc and voided, $\rho_{LOCA} = 0.001$ g/cc) for three different burn-up states (0, 4 and 8 GWd/TU) at operating temperatures. For these six cases, the numerical results, though not exhaustive, indicate that EVENT can achieve comparable levels of accuracy as MCNP in calculating the eigenvalue and the fuel pin fission density at a competitive computational effort. This gives confidence in applying EVENT to transient analyses at the fuel pin level in a selected part of a CANDU core such as the limiting bundle during a LOCA.

Earlier, it was found that HELIOS with the 45-group neutron cross section library (with no adjustments to the ^{238}U resonance capture) distributed with the *HELIOS System* 1.6 (ref. 4) agrees well with MCNP in calculating the coolant void reactivity in a single CANDU cell with 37 fuel pins. Therefore, it is reasonable to expect that the combined code system EVENT/HELIOS will be accurate enough for transient and static studies in CANDU configurations.

I. MODELING DESCRIPTION

The benchmark configuration used in this study is based on a typical square lattice cell with a single CANDU cluster taken from ref. 5. A quarter of the lattice cell is shown in Figure 1. The cell consists of a pressure tube filled with heavy water coolant, a helium filled gap, and a calandria tube surrounded by heavy water moderator. Both coolant and moderator contain a small amount of light water impurity. The cluster contains 37 fuel rods made from natural UO_2 and a Zircaloy cladding. In all cases, operating temperatures are used.

For the two coolant states that are typical of the hot operating condition and the voided (LOCA) condition, the coolant is assumed to be uniformly distributed inside the pressure tube. Results are given for fresh fuel, mid-burnup (4 GWd/tU), and high burnup (8 GWd/tU) depletion states. In both MCNP and EVENT, the three-dimensional cell was modeled as finite in the horizontal direction (along the pressure-tube axis). Specular reflection was used on all external surfaces of the cell. No approximations were made in MCNP with respect to the geometry of the model.



1. Moderator
2. Calandria Tube
3. Gap
4. Pressure Tube
5. Fuel Rod
6. Coolant

Figure 1. Typical CANDU Lattice Cell

II. GEOMETRY MODELING WITH EVENT

The finite element mesh used in all the calculations is presented in Figure 2. It consists of a mixture of 5623 linear triangles and bi-linear quadrilaterals, totaling 2980 nodes. This mesh is judged to be sufficiently fine to ensure spatial convergence of the solution. The Pressure tube/Calandria tube gap, which consists of Helium, is not explicitly meshed; instead a ray tracing method is used to couple the pressure tube and Calandria regions [see ref 2].

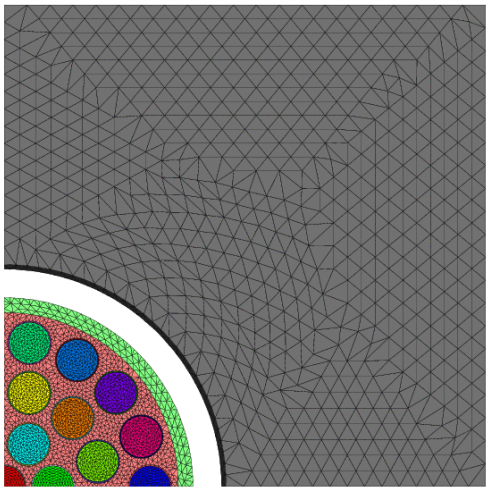


Figure 2. Finite Element Representation of CANDU Lattice Cell

The use of ray tracing is an acceptable approximation to the Helium cross-sections which are relatively small. The radius of the fuel pins is adjusted in order to conserve the fissile mass (in this case fissile mass is conserved to five decimal place accuracy). Reflective boundary conditions are used to take advantage of the inherent symmetry for this cell problem.

III. CROSS SECTION LIBRARIES

The 45-group cross sections used in both codes were generated using HELIOS-1.6 in which the cell was modeled in two-dimensional geometry with small approximations in the geometry of the pressure tube, gap, and calandria tube as described in ref. 4. These approximations had a negligible effect on the transport calculation. A specular reflection boundary condition was used on the external boundaries of the cell.

Fuel cross sections were generated at 0 and 100% coolant void fractions for the 0, 4, and 8 GWd/tU burnup levels. All other cross sections were generated at 0% coolant void fraction and 0 GWd burnup.

Due to the spatial self-shielding corrections performed in HELIOS, the cross sections associated with a given material will, in general, be different in different computational meshes. The non-fuel cross sections were generated by homogenizing the cross sections from all of the individual computational regions associated with a single material. Fuel materials were homogenized within each of the four annuli.

FORTRAN codes were written to convert ZENITH output to MCNP's ACE format and to GEM format for EVENT. Since the method for defining P_1 scattering cross sections in ACE format is not straightforward, transport-corrected total and P_0 scattering matrices were used (as in HELIOS), with the transport correction defined as

$$\Sigma_{tc,g} = \Sigma_{ab,g} + \sum_{g'} \Sigma_{s0,g\to g'} - \Sigma_{tr,g} \tag{1}$$

The quantities with subscripts *tr* and *s0* denote the transport and un-corrected P_0 cross sections, respectively.

The treatment of (n,2n) and (n,3n) reactions in HELIOS-1.6 may lead to negative absorption cross sections in a few of the highest energy groups. Also, the use of the transport correction in the P_0 scattering matrices may lead to negative self-scattering cross sections.

Since MCNP interprets cross section ratios as probabilities, negative cross sections cannot be tolerated. Any negative absorption or self-scattering cross sections in the ZENITH output was replaced with zero values, and the corresponding difference added to the transport cross section. No negative cross sections were noticed for fuel materials.

Since the library contains macroscopic cross sections, the number densities on cell and material cards should be set to 1, except for coolant when it has a density other than the one corresponding to the hot operating condition (HOC, $\rho_{HOC} = 0.80623\,\text{g/cc}$). In general, the coolant's number density will be set to

$$ND = \frac{\rho}{\rho_{HOC}} \tag{2}$$

IV. RESULTS

The benchmark results were obtained using the Monte Carlo transport code MCNP4C with the multigroup option and the 45-group HELIOS generated library.

For eigenvalue (multiplication constant) calculations, 125 million active histories were run in MCNP for each of the six cases to obtain a statistical (absolute) error of less then 10 pcm. The EVENT results quoted are for a P_9 angular approximation. Both the MCNP and EVENT results are listed in TABLE I.

TABLE I. Eigenvalue Comparison

Case	MCNP	σ	EVENT	Δk [1)]
HOC, 0 GWd	1.11326	0.00008	1.11256	-0.00070
HOC, 4 GWd	1.04625	0.00007	1.04511	-0.00114
HOC, 8 GWd	0.98072	0.00007	0.97930	-0.00142
VOID, 0 GWd	1.13562	0.00008	1.13428	-0.00134
VOID, 4 GWd	1.06358	0.00007	1.06208	-0.00150
VOID, 8 GWd	0.99574	0.00007	0.99428	-0.00146

[1)] $\Delta k = k_{EVENT} - k_{MCNP}$

The fuel pin fission density distribution from EVENT was compared to that from MCNP. The comparison was performed for HOC at 4GWd/TU. The MCNP results were obtained with 25 million active histories to obtain statistical errors of less than 0.05% in each pin. A flux tally for reaction –2 (multigroup fission) was performed for each fuel pin.

The pin fission rate results normalized to the total number of pins in the quarter cell are summarized in TABLE II. The MCNP statistical error is relative. The fuel pins are numbered clockwise starting azimuthally from the vertical axis, and then radially outward for each of the four annuli. One can note the uniform distribution of the fission rate in each annulus.

The results show a consistent under-prediction of the eigenvalue by EVENT by approximately 100-150 pcm. This seems to indicate the presence of some form of

systematic effect, which reduces the predicted reactivity of the configurations. This effect could be due to the poor tolerance tuning of the various interlinked iterative schemes (Power, up-scattering, ray tracing, and Preconditioned Conjugate Gradients for the system of equations for the angular moments of the flux at each finite element node) or insufficient angular resolution. Further research is apace to help to track down the cause of these discrepancies.

TABLE II. Fuel Pin Fission Rate Comparison

Pin #	MCNP	σ[1)]	EVENT	Error[2)]
1	0.77860	0.06	0.77495	-0.47
2	0.82028	0.04	0.81569	-0.56
3	0.81999	0.03	0.81571	-0.52
4	0.93208	0.03	0.92734	-0.51
5	0.93171	0.03	0.92358	-0.87
6	0.93134	0.03	0.92377	-0.81
7	1.15743	0.04	1.15834	0.08
8	1.15672	0.03	1.16769	0.95
9	1.15777	0.03	1.16529	0.65
10	1.15744	0.03	1.16407	0.57
11	1.15665	0.03	1.16133	0.40

[1)] relative statistical error, percent
[2)] relative error calculated as 100*(EVENT-MCNP)/MCNP

V. DISCUSSION AND CONCLUSIONS

The applicability of the transport theory code EVENT was assessed for analyses of CANDU lattice cell by comparing the EVENT eigenvalue and fuel pin fission density distribution to the corresponding values obtained with the Monte Carlo transport code, MCNP. Both codes used the same 45-group cross sections generated by HELIOS.

We have found that EVENT is capable of reproducing the MCNP eigenvalue within 150pcm. The pin fission rates obtained with EVENT are less than 1% from MCNP values. As mentioned above, the EVENT calculations have not been exhaustive in that detailed fine-tuning of tolerances and fully converged angular resolution were not attempted. The results of these first tests show that transport calculations with MCNP accuracy can be performed using EVENT at a competitive computational price. This implies that an EVENT/HELIOS code package could be used with confidence for 3-D calculations in CANDU configurations for transient analyses at fuel-pin level in a selected part of the core such as the limiting bundle during a LOCA.

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