Comparative Static Simulations of a CANDU6 Cell Using Different Transport Codes

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Abstract

The solution of the time dependent Boltzmann equation remains quite a challenge. We are in the process of developing such a method using the stochastic Monte Carlo approach for two reasons: First, at the cell level, we will be able to obtain time dependent homogenized cross sections for use in full core diffusion calculations. Second, the Monte Carlo methods are scalable to perform full core if and when appropriate computer resources become available.
The Time dependent approach will be concretized a new module that will be added to an existing Monte Carlo code. As a first step towards this goal, we need to choose the initial Monte Carlo code to be used as start point. For this reason, we have compared results concerning the void reactivity of a fresh fuel CANDU6 cell, using two Monte Carlo codes, namely VTT developed SERPENT and MIT developed OpenMC together with the deterministic DRAGON code. Several libraries are used in this comparison. We conclude that OpenMC is a good candidate for implementation of a time dependent simulation.

1. Introduction

The main purpose of our research concerning nuclear power plants is to develop an approach to efficiently predict the behavior of the reactor core and components during a transient. It is still difficult to modelize and simulate the entire reactor core with fine details using the transport equation. The approach is then to solve the Boltzmann equation for a small region of the reactor, such as a singe cell containing one bundle, to obtain spatially homogenized and energy-condensed properties. Following this, a diffusion simulation is performed to obtain the flux distribution over the entire core.

Numerous methods have been developed to solve the Boltzmann equation. They can be classified in two major groups: the deterministic and the stochastic (Monte Carlo).

The DRAGON code [1] is one of the deterministic codes that are used to obtain the reactor databases. It uses collision probability method in 2D and 3D. Furthermore, it can also use the Method Of Characteristics (MOC) or the **Sn** methods to solve the transport equation.

MCNP [2], Serpent [3], OpenMC [4], TRIPOLI [5] are Monte Carlo codes that also solve the transport equation.

Results obtained using those software are used in diffusion codes, such as DONJON [6], to estimate the behavior of the entire reactor core. Here, DRAGON, OpenMC, and Serpent are used to obtain databases for a CANDU6 reactor cell. We then get the homogenized cross sections for a voided

CANDU6 cell. Reactivity of void will be calculated and discussed. Finally, we will discuss the interest in using OpenMC for a CANDU6 reactor.

2. Theory

The body text of the paper contains headings, subheadings, pictures, diagrams, tables, figures, formulae and other relevant information. Section headings should be in bolded 12 point The most important result in the transport step is producing the macroscopic condensed and homogenized cross sections for the reactor cell. Three steps are needed to achieve this objective. First, obtain the flux distribution, which is the solution of the condensed and integrated transport Boltzmann equation:

$$\Sigma_{t,g}(\vec{r},t)\phi_g(\vec{r},t) + \nabla.J_g(\vec{r},t) = \sum_{g'=1}^{G}\Sigma_{s,g\leftarrow g'}(\vec{r},t)\phi_{g'}(\vec{r},t) + \frac{1}{K_{eff}}\chi_g\sum_{g'=1}^{G}\nu_{g'}\,\Sigma_{f,g'}(\vec{r},t)\phi_{g'}(\vec{r},t) \quad (1)$$

Second, obtain the homogenized and condensed flux by:

$$\phi_{m,h} = \frac{1}{V_m}\sum_{g\in(G\cap H)}\sum_{i\in(N\cap M)} V_i\phi_{i,g} \quad (2)$$

(where V_m is the sum of all micro volumes "i" in the cell $V_m = \sum_{i\in(N\cap M)} V_i$.N is total number of micro volumes and M is the total number of macro volumes)

And finally, get the homogenized cross sections:

$$\Sigma_{x,m,h} = \frac{1}{V_m\phi_{m,h}}\sum_{g\in(G\cap H)}\sum_{i\in(N\cap M)} V_i\phi_{i,g}\;\Sigma_{x,i,g} \quad (3)$$

(where H is the total number of macro group of energy and G is the number of micro group of energy)

In a LOCA accident, the voided channels in CANDU6 lead to the coolant void reactivity:

$$\Delta\rho = \rho_{\text{voided}} - \rho_{\text{cooled}} = \frac{K_{eff}(\text{voided}) - K_{eff}(\text{cooled})}{K_{eff}(\text{cooled})\times K_{eff}(voided)}$$

Here, results obtained by different transport codes will be discussed but will not detail the physical reasons for the coefficient. The physical phenomena related to the void coefficient values for a CANDU6 lattice cell are discussed in many published articles [7].

3. CANDU6 Reactor Modeling

The CANDU6 reactor is fuelled with natural uranium. Moderator, reflector and coolant are constituted of heavy water D_2O. The pressurized coolant circuit is separated from the moderator- reflector. The lattice cell contains a bundle of 37 fuel pins surrounded by coolant and separated from the moderator by pressure and calandria tubes (Figure 1). The temperature of the coolant is 290 °C, whereas the moderator is 70 °C.

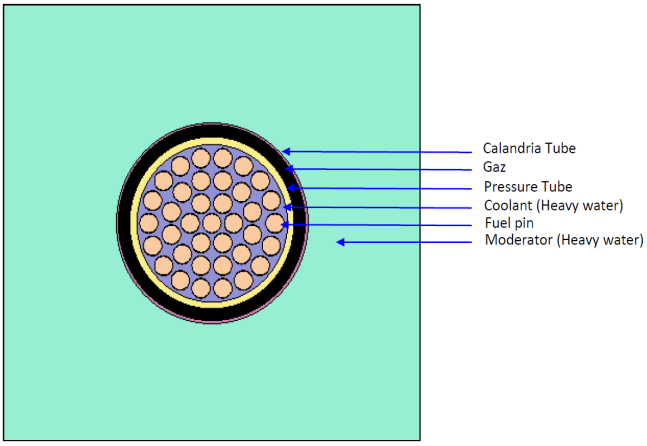

Figure 1 CANDU6 reactor cell

As discussed before, the first step in the reactor modeling chain is solving the transport equation and obtaining the database for the reactor simulation.

Using a deterministic code such as DRAGON, one must use multi-group cross sections obtained by running the NJOY code [8]. There are numerous cross sections data libraries such as ENDF-B or Jeff, using various energy meshes: X-MAS-177 (defined jointly by UK and France), SHEM281 (N. Hfaiedh and A. Santamarina) [9] or SHEM295 (Alain Hébert) [10] etc., and numerous formats of library files such as DRAGLIB for DRAGON code, WIMSLIB for DWIMS or WIMS code, and IAEA for WIMS.

In the Monte Carlo approach, continuous energy data cross sections are used. There is only one available format, the *ACE-format*, as defined by MCNP developers. OpenMC, Serpent and MCNP use the same files but each creates his own index file for individual nuclide data.

Only DRAGON, Serpent and OpenMC will be used here and their versions are listed in the table 1.

Both DRAGON and OpenMc were developed using Fortran programming language. DRAGON was initially developed using Fortran77, however DRAGON5 is up to date with Fortran2003. Released in 2012, OpenMC is the newest transport code used. It was developed using Fortran2003 also. On the other hand, Serpent uses C/C++ language.

DRAGON data results are written in a "*compo*" file used directly by the diffusion code, DONJON. Therefore, the Monte Carlo results have to be transformed into a " *compo*" format file if to be used by DONJON.

	Version
DRAGON	5.0.0
Serpent	1.1.19
OpenMC	0.5.3

Table 1 Codes version

4. Deterministic Transport Results

DRAGON is the deterministic lattice code that was used to solve the multi-group transport Boltzmann equation for a CANDU6 cell. The two-dimensional collision probability method was chosen. ENDFB7 and JEFF3.1.1 are the cross sections libraries used for this study. The format of libraries is DRAGLIB. Fresh fuel composition materials are chosen. For the voided cell, the coolant was replaced by void (density equal to zero).

DRAGON contains two different tracking modules, NXT and EXCELT [11]. The EXCELT module allows only simple geometries in single precision and tracking lines in double precision. However, NXT is a newer module using double precision for both geometry description and tracking lines and is able to deal with more complex geometries. Table 2 and 3 present the k_{eff} using EXCELT and NXT modules for a CANDU6 cell.

DRAGON		XMAS-172	SHEM-281	SHEM-295	SHEM-315	SHEM-361
Cooled CANDU6 cell	endfb7	1.120501	1.121469	1.123489	1.123617	1.123449
	Jeff 3.1.1	1.118341	1.119294	1.121263	1.121389	1.12122
Voided CANDU6 cell	endfb7	1.143286	1.144173	1.1463	1.146444	1.146248
	Jeff 3.1.1	1.141095	1.141966	1.144044	1.144188	1.143988
Δk_{eff}	endfb7	0.022785	0.022704	0.022811	0.022827	0.022799
	Jeff 3.1.1	0.022754	0.022672	0.022781	0.022799	0.022768
ρ perturbation	endfb7	0.017786	0.017694	0.017713	0.017721	0.017705
	Jeff 3.1.1	0.01783	0.017738	0.017759	0.017769	0.01775

Table 2 k_{eff} and reactivity for a **CANDU6** cell using module **EXCELT** module for tracking**.**

5. Monte Carlo Transport Results

In the Monte Carlo simulations, we used 3000 batchs each with 10^5 particles. The first 150 batch results were ignored in tallies process. We have chosen to use ENDFB7 and JEFF3.1.1 for those simulations to compare results with previous deterministic simulations. The same libraries cross-sections files were used for all Monte Carlo codes.

DRAGON		XMAS-172	SHEM-281	SHEM-295	SHEM-315	SHEM-361
Cooled CANDU6 cell	endfb7	1.120499	1.121465	1.123484	1.123611	1.123444
	Jeff 3.1.1	1.118344	1.119288	1.121258	1.121383	1.121215
Voided CANDU6 cell	endfb7	1.14329	1.144183	1.146311	1.146455	1.14626
	Jeff 3.1.1	1.141101	1.141976	1.144055	1.144199	1.144001
Δk_{eff}	endfb7	0.022791	0.022718	0.022827	0.022844	0.022816
	Jeff 3.1.1	0.022757	0.022688	0.022797	0.022816	0.022786
ρ perturbation	endfb7	0.017791	0.017705	0.017725	0.017734	0.017718
	Jeff 3.1.1	0.017833	0.01775	0.017772	0.017782	0.017764

Table 3 k_{eff} and reactivity for a **CANDU6** cell using module **NXT** module for tracking**.**

5.1 SERPENT Simulation for a CANDU6 Cell

Serpent is a Monte Carlo continuous energy reactor physics code. The code development started at the VTT Technical Research Centre of Finland in 2004. It can perform eigenvalue simulations, fixed source simulations and burnup calculations. Results of CANDU6 cell simulations using Serpent are presented in table 4.

5.2 OpenMC Simulations for a CANDU6-Cell

OpenMC is a recent Monte Carlo *open source* code developed by the CRPG group of the Massachusetts Institute of Technology (MIT). OpenMC was first released in 2012. It is a full toolkit with different features and approaches such as using XML as input files, using Coarse Mesh Finite Difference method (CMFD) for accelerating convergence, parallel tracking based on neighbors approach, etc. OpenMC is able to perform eigenvalue calculations, fixed sources simulations. However, the isotopic evolution is not yet included. Table 5 presents results obtained using OpenMC.

SERPENT		k_{eff} analog	+/-	k_{eff} implicit	+/-
Cooled CANDU6 cell	endfb7	1.12393	0.0004	1.12347	0.0001
	Jeff 3.1.1	1.12221	0.0004	1.12173	0.00011
Voided CANDU6 cell	endfb7	1.14065	0.00041	1.14063	0.0001
	Jeff 3.1.1	1.13894	0.0004	1.13856	0.0001
Δk_{eff}	endfb7	0.01672		0.01716	
	Jeff 3.1.1	0.01673		0.01683	
ρ perturbation	endfb7	0.013042		0.013391	
	Jeff 3.1.1	0.013089		0.013178	

Table 4 k_{eff} for a cooled and voided **CANDU6** cell using **Serpent**

OpenMC		K_{eff} Collision	K_{eff} Track-length	K_{eff} Absorption	Combined K_{eff}
Cooled CANDU6 cell	endfb7	1.1233	1.12345	1.12355	1.12345
	+/-	0.00037	0.00041	0.00035	0.00028
	Jeff 3.1.1	1.12154	1.12149	1.12231	1.12196
	+/-	0.00038	0.00042	0.00035	0.00028
Voided CANDU6 cell	endfb7	1.14114	1.14133	1.14025	1.14064
	+/-	0.00038	0.00041	0.00033	0.00026
	Jeff 3.1.1	1.13776	1.13789	1.13876	1.13831
	+/-	0.00037	0.0004	0.00034	0.00027
Δk_{eff}	endfb7	0.01784	0.01788	0.0167	0.01719
	Jeff 3.1.1	0.01622	0.0164	0.01645	0.01635
ρ perturbation	endfb7	0.013917	0.013944	0.013035	0.013414
	Jeff 3.1.1	0.012711	0.012851	0.012871	0.0128021

Table 5 k_{eff} for a cooled and voided fresh **CANDU6** cell using **OpenMC**

6. Comparing Homogenized Cross Sections

It is necessary to compare nuclear parameters other then the k-effective and void reactivity. These would be the condensed and homogenized cross sections to be used in the diffusion process. Tables 6 and 7 present the variation of the total, absorption, scattering and fission cross-sections between OpenMC and Serpent for both cooled and voided CANDU6 cell.

7. Results Analysis

Before starting analyzing the results of different transport codes, let us look at the neutronic role of the coolant in the CANDU6 reactor. With about 83% of the volume cell constituted by the moderator and only 4% by the coolant, the moderating and absorption properties of the coolant appears to be small compared to those of moderator. For example, only about 0,03% of absorptions occur in the coolant region [7]. The coolant region causes the down scattering of fast neutrons just produced by fissions and up-scattering for neutrons that are almost thermalized by the moderator. The net neutronic role of the coolant is thus to decrease the cell reactivity and decrease the reactor power. The absence of coolant introduces an increase of power and a positive reactivity.

To compare results from different codes, it is important to take into account the differences in the development approaches of lattice codes.

Four major reasons can explain the differences shown in the results:

1. The use of different databases is the most important difference between codes. The deterministic transport code DRAGON uses multi-group cross sections obtained by NJOY. In this case, only the multi-group transport equation can be solved, including self-shielding, to

obtain accurate results. In the case of Monte Carlo simulation, the cross sections database used is continuous in energy that do not need any preprocessing and any self-shielding.

2. The second difference is based on the solving process of the transport equation. The transport equation in multi-group form is solved by DRAGON using the collision probability method. However, in Monte Carlo codes, an important number of particles are followed, one by one, to predict the general behavior of all particles.
3. The gap between the Monte Carlo and the deterministic simulations is accentuated by the differences in the temperatures in the materials geometry. Monte Carlo codes use continuous cross sections for each nuclide but only with six fixed different temperatures (300°K, 600°K, 900°K, 1200°K, 1500°K, 180°K). However, DRAGON uses multi-group cross sections for different temperatures and proceeds with an interpolation process to obtain the cross sections for the exact temperature.
4. Finally, differences between OpenMC and Serpent can be explained by the tracking approach used by each code. OpenMC follows particles between two collisions and tracks are sampled using the total cross section of the material traversed by the particle. At surfaces between two materials, particles are stopped and new tracks are sampled using the new cross sections. However, Serpent uses the ***delta tracking*** approach [12] where particles are stopped only at boundaries of the geometry. Tracks are then sampled using the largest total cross section value of all materials present in the geometry.

			Serpent ENDF-B7	**OpenMC** ENDF-B7	ΔΣ	**Serpent** Jeff3.1.1	**OpenMC** Jeff3.1.1	ΔΣ
Homogenized Cross Sections for the cell	Fast Gr	Total XS	3.16E-01	3.16E-01	0.00E+00	3.19E-01	3.16E-01	-3.00E-03
		Absorption XS	1.77E-03	1.77E-03	0.00E+00	1.67E-03	1.77E-03	1.00E-04
		Scattering XS	3.15E-01	3.15E-01	0.00E+00	3.14E-01	3.14E-01	0.00E+00
		Fission XS	3.38E-04	3.38E-04	0.00E+00	3.30E-04	3.36E-04	6.00E-06
	Thermal Gr	Total XS	4.19E-01	4.19E-01	0.00E+00	4.22E-01	4.18E-01	-4.00E-03
		Absorption XS	3.19E-03	3.19E-03	0.00E+00	3.29E-03	3.20E-03	-9.00E-05
		Scattering XS	4.16E-01	4.16E-01	0.00E+00	4.19E-01	4.15E-01	-4.00E-03
		Fission XS	1.61E-03	1.61E-03	0.00E+00	1.67E-03	1.61E-03	-6.00E-05
Homogenized Cross Sections for the moderator	Fast Gr	Total XS	3.33E-01	3.33E-01	0.00E+00	3.36E-01	3.34E-01	-2.00E-03
		Absorption XS	2.94E-05	2.94E-05	0.00E+00	2.89E-05	3.20E-05	3.10E-06
		Scattering XS	3.33E-01	3.33E-01	0.00E+00	3.36E-01	3.33E-01	-3.00E-03
		Fission XS	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
	Thermal Gr	Total XS	4.37E-01	4.37E-01	0.00E+00	4.41E-01	4.37E-01	4.00E-03
		Absorption XS	3.60E-05	3.60E-05	0.00E+00	3.71E-05	3.60E-05	1.10E-06
		Scattering XS	4.37E-01	4.37E-01	0.00E+00	4.41E-01	4.37E-01	-4.00E-03
		Fission XS	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Table 6 Homogenized cross sections obtained by **OpenMC** and **Serpent** codes for a fresh fueled CANDU6 cell

			Serpent ENDF-B7	**OpenMC** ENDF-B7	ΔΣ	**Serpent** Jeff3.1.1	**OpenMC** Jeff3.1.1	ΔΣ
Homogenized Cross Sections for the cell	Fast Gr	Total XS	3.01E-01	2.98E-01	-3.00E-03	3.01E-01	2.98E-01	-3.00E-03
		Absorption XS	1.52E-03	1.59E-03	7.00E-05	1.52E-03	1.59E-03	7.00E-05
		Scattering XS	2.97E-01	2.96E-01	-1.00E-03	2.97E-01	2.96E-01	-1.00E-03
		Fission XS	3.38E-04	3.43E-04	5.00E-06	3.35E-04	3.40E-04	5.00E-06
	Thermal Gr	Total XS	4.13E-01	4.09E-01	-4.00E-03	4.13E-01	4.09E-01	-4.00E-03
		Absorption XS	3.35E-03	3.25E-03	-1.00E-04	3.36E-03	3.26E-03	-1.00E-04
		Scattering XS	4.10E-01	4.06E-01	-4.00E-03	4.09E-01	4.06E-01	-3.00E-03
		Fission XS	1.70E-03	1.64E-03	-6.00E-05	1.71E-03	1.64E-03	-7.00E-05
Homogenized Cross Sections for the moderator	Fast Gr	Total XS	3.35E-01	3.32E-01	-3.00E-03	3.35E-01	3.32E-01	-3.00E-03
		Absorption XS	2.81E-05	3.11E-05	3.00E-06	3.06E-05	3.39E-05	3.30E-06
		Scattering XS	3.35E-01	3.32E-01	-3.00E-03	3.35E-01	3.32E-01	-3.00E-03
		Fission XS	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
	Thermal Gr	Total XS	4.41E-01	4.37E-01	-4.00E-03	4.41E-01	4.37E-01	-4.00E-03
		Absorption XS	3.71E-05	3.58E-05	-1.30E-06	3.71E-05	3.58E-05	-1.30E-06
		Scattering XS	4.41E-01	4.37E-01	-4.00E-03	4.41E-01	4.37E-01	-4.00E-03
		Fission XS	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Table 7 Homogenized cross-sections obtained by **OpenMC** and **Serpent** codes for voided CANDU6 cell

8. Conclusion

We find that stochastic and deterministic methods converge in their results. We can also conclude also that OpenMC could be used for CANDU6 cell simulations to obtain homogenized and condensed cross sections for diffusion calculations since results are similar to those obtained by other codes.

In this study, we have presented the behavior of the reactor after a 100% instantaneous removal of coolant from the fuel channel. This conservative approach is used in most reactors LOCA analysis. However the time dependence of partial voiding is still neglected and is under investigation.

Due to the open source licensing of OpenMC, its use of modern approach of programming with FORTRAN-2003, and for the good agreement with Serpent results, we decided to use OpenMC for the next steps in solving the time dependent Boltzmann equation. This will be the basis of the adiabatic assumption analysis of a transient situation in a nuclear reactor core.

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