MODELS FOR RESONANCE SELF-SHIELDING CALCULATION IN NEUTRONIC ANALYSIS OF THE CANDU-SCWR FUEL CHANNEL

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Abstract

We present the complete CANDU-SCWR model developed for the DRAGON code. A particular attention is brought to the development of the geometries used for resonance self-shielding calculations in the cases of single lattice and 2x2 assembly simulations. The study of the multiplication constant has shown that it is possible to use a simplified geometry for the resonance self-shielding calculation in assembly calculations. Finally, comparisons of the multiplication constant, neutron spectra and reaction rates obtained for different lattice pitches have demonstrated the importance of radiative captures in ^{238}U resonances.

1. Introduction

Generation IV nuclear reactors are currently in development worldwide under the Generation IV International Forum (GIF) [1]. These reactors will present several technological innovations in order to improve resources management and proliferation resistance, to ensure safety and reliability and to reduce construction and operating costs. The GIF has selected three fast reactors and three thermal reactors: the gas-cooled, the sodium-cooled and the lead-cooled fast reactors, the very-high-temperature reactor, the molten salt reactor and the Supercritical Water-Cooled Reactor (SCWR).

By operating at temperatures and pressures above the thermodynamic critical point of water (374°C and 22.1 MPa), both the pressure vessel and pressure tube versions of the SCWR will reach a thermal efficiency of about 40-45% compared to 33-35% for the current generation (2^{nd}) of nuclear reactors [2]. The pressure tube version of the SCWR considered in this paper is a natural evolution of the CANDU reactors and is also called CANDU-SCWR. Its reference design has an operating pressure of 25 MPa, a reactor inlet temperature of 350°C and a reactor outlet temperature of 625°C [3]. The CANDU-SCWR will be used to produce electricity, hydrogen and drinking water and will also serve as a heat source depending on the needs [4].

Two types of CANDU-SCWR fuel channel are currently in development: the re-entrant type and the insulated type [5]. In the re-entrant fuel channel, the fuel bundle is contained within (from the inner to the outer) an inner tube, a pressure tube and a calandria tube. The calandria tube is in direct contact with the moderator. A gas isolates the calandria tube from the pressure tube. Prior to flow through fuel bundles, the coolant must pass between the pressure and the inner tubes. In the insulated fuel channel, also called High Efficiency fuel Channel (HEC), the fuel bundle, which is immersed in the coolant, is contained (from the inner to the outer) within a perforated liner, a segmented insulator and a pressure tube. The pressure tube is thermally insulated from the coolant and is in direct contact with the moderator. In this configuration, the coolant pressure is transmitted to the pressure tube through the segmented and perforated zones. The liner protects the insulator from erosion

caused by the circulation of coolant and from the movement of fuel bundles during on-line refueling. This paper focuses on the analysis of this last fuel channel.

In lattice calculations, the resonance self-shielding calculations are performed to correct the microscopic cross sections associated with heavy (resonant) isotopes in the energy groups dominated by these resonances. Such a correction is required in order to take into account of the depressions in the weighting flux in this region. The resonance self-shielding calculation is generally separated from the main flux calculation. In practice, these two calculations are performed on different geometries [6]. The DRAGON [7] resonance self-shielding model selected corresponds to the `SHI:` module and is based on rational expansions of fuel-to-fuel collision probabilities [8]. In the model, the number of terms involved in these expansions will differ depending on the specific self-shielding correction option selected. Here, three options will be considered: 1) the original Stamm'ler model, 2) the Stamm'ler model with the Nordheim approximation and 3) the Stamm'ler model with the Nordheim approximation and Riemann integration.

In section 2, of this paper we present the geometries of the CANDU-SCWR lattice cell developed in DRAGON for the main flux and the resonance self-shielding calculations. From these two geometries, we have evaluated the effect of the lattice pitch on k_∞, on the neutron flux and on some reaction rates. This will be followed in section 3, by a presentation of the different models developed for the resonance self-shielding calculation in the case of a 2x2 assembly of CANDU-SCWR lattice cells in checkerboard pattern.

2. Description of the CANDU-SCWR lattice cell model and simulation results

Here the analysis will be performed using the `NXT:` tracking module of DRAGON 3.06. In all cases, the collision probability (CP) method will be used to solve the neutron transport equation. Only infinite multiplication constant problems (without neutron leakage) will be considered. The 69 groups microscopic cross sections library selected for our calculations is the "iaea" WIMS-D4 library from WLUP [9].

Since we are using the CP approximation, one must select carefully the spatial mesh discretization (radial and Cartesian) in order to ensure constant sources and constant flux over spatial regions of the geometry. On the other hand it is generally possible to use a simplified version of this geometry for the resonance self-shielding calculation.

Here we will first discuss how the optimized geometries used respectively for the main flux and the resonance self-shielding calculations were selected. We will then evaluate the effect of the lattice pitch on the infinite multiplication constant k_∞, on the average neutron flux and on the absorption reaction rates.

2.1 CANDU-SCWR geometries

In this study, the CANDU-SCWR lattice cell is composed of a 43 elements CANFLEX® fuel bundle and of a HEC fuel channel as shown in Figure 1a.

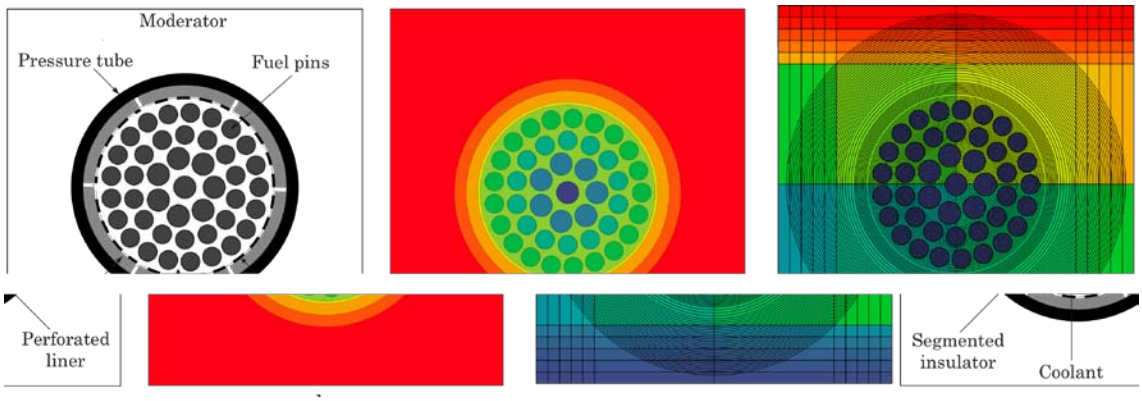

Figure 1 CANDU-SCWR lattice cell (a) as modeled in DRAGON (b) and with the spatial mesh discretization optimized for the main flux calculation (c)

As shown in Figure 1b, it is not possible to define segmented and perforated regions in DRAGON. Thus, in our models, the insulator and the liner regions contain, respectively, 70% and 45% of light water (at the coolant pressure and temperature). Table 1 presents the main elements of the geometries.

Table 1 Description of the CANDU-SCWR geometries in DRAGON

Description	**Value**
Coolant	Light water
Fuel rings (from the inner to the outer)	1, 7, 14 and 21 pins/ring
43 fuel elements material	UO_2
Fuel enrichment	4.25 wgt%
Fuel sheath material	Stainless Steel
Liner material	Stainless Steel
Liner porosity	45%
Insulator material	ZrO_2
Insulator porosity	70%
Pressure tube material	EXCEL (Zr alloy)
Moderator	Heavy water
Lattice pitch	Variable from 21 cm to 28 cm

2.1.1 Geometry for main flux calculation

The construction and the validation of the geometry used for main flux calculation have been presented in details in a previous publication [10]. As shown in Figure 1c, the optimized radial mesh discretization results in the fuel pins, the fuel sheaths, the coolant, the liner, the insulator, the pressure tube and the moderator regions being subdivided radially into 8, 1, 50, 1, 8, 4 and 25 sub-regions respectively. The optimized Cartesian mesh discretization depends on the lattice pitch as shown in Table 2. Here S and N are respectively the total number of surfaces and sub-regions present in the geometry after the spatial mesh discretization has been applied.

Table 2 Cartesian mesh discretization optimization

Pitch (cm)	**Cartesian mesh discretization (squares per corner)**	***S* (surfaces)**	***N* (sub-regions)**
21	25	48	1016
24	64	72	1196
28	121	96	1448

In the CP method, a tracking process is applied over the entire geometry in order to cover a sufficiently large number of trajectories followed by neutrons. Here, the optimized tracking parameters consist of 50 equidistant angles in the range [0, π] and of 63 parallel lines per centimeter. This is consistent with the requirements that the numerical integration errors on the volumes and the surfaces are lower than 1.0% when compared with the exact values.

2.1.2 Geometry for resonance self-shielding calculation

Generally, the geometry used for resonance self-shielding calculation does not require a very fine spatial mesh discretization. In order to validate this practice, we have compared neutronic parameters obtained from geometries with and without the optimized spatial mesh discretization (as described in section 2.1.1 for a pitch of 21 cm). In all cases, the geometry used for the main flux calculation is that presented in Figure 1c. Isotropic reflection boundary conditions have been applied uniformly on all the external surfaces for all the geometries. The neutronic parameters studied are presented in Table 4. The cross sections have been condensed to two energy groups with the cutoff energy at 0.625 eV and homogenized over the entire cell (group 1 is the fast group and 2 the thermal group).

Table 3 Neutronic parameters used to validate the geometry for resonance self-shielding calculation

Neutronic parameters	**Description**
k_∞	Infinite multiplication constant
$\nu\Sigma_f^1$ and $\nu\Sigma_f^2$	Product of the average number of neutrons produced per fission with the fission cross section for group 1 and 2
Σ^1 and Σ^2	Total cross section for group 1 and 2
$\Sigma_s^{1\to1}$, $\Sigma_s^{1\to2}$, $\Sigma_s^{2\to1}$ and $\Sigma_s^{2\to2}$	Scattering cross section from initial (i) to final (f) group ($i \to f$)

This study was performed for fresh fuel and for the first and the twelfth fuel bundle in a 594 cm long CANDU-SCWR fuel channel. Table 5 presents the local properties found in the center of these fuel bundles [11].

Table 4 Local properties used to validate the geometry for resonance self-shielding calculation

Fuel bundle	**Fission power (kW)**	**Coolant temperature (K)**	**Coolant density (g/cm^3)**
1^{st}	82	663	0.215
12^{th}	82	888	0.069

We observe that the effect of the spatial mesh discretization for resonance self-shielding calculation is weak for k_∞ (a maximum difference of 0.3262 mk) and negligible for the macroscopic cross sections (a difference of less than 0.01 %). In the case of k_∞, this difference is acceptable because in finite reactor calculation, uncertainty on k_∞ can reach values of 2-3 mk.

From these results and considering the fact that the computing time associated with resonance self-shielding calculation is about 5 times longer than that required for the main flux calculation, we conclude that the geometry used for resonance self-shielding calculation does not require a very fine spatial mesh discretization in this case.

2.2 Evaluation of the effect of the lattice pitch

The effect of the lattice pitch has been assessed for three different cell types (different coolant density). Table 6 presents the local properties used for this study. These properties have been obtained from a coupled neutronic/thermal-hydraulics analysis of the CANDU-SCWR fuel channel with fresh fuel [12].

Table 5 Local properties used for the evaluation of the effect of the lattice pitch

Lattice cell	Fission power (kW)	Coolant temperature (K)	Coolant density (g/cm^3)
C1	994	666	0.615
C2	994	666	0.345
C3	994	666	0.074

The coolant densities of C1 and C3 represent the values averaged over the first and the twelfth fuel bundle respectively. The coolant density of C2 is the average coolant density of C1 and C3. The other properties (fission power and coolant temperature) represent the values averaged over the sixth fuel bundle where the fission power is at a maximum in the fuel channel.

Table 6 DRAGON k_∞ for CANDU-SCWR fresh fuel

Lattice pitch (cm)	k_∞		
	C1	C2	C3
21	1.3389	1.3427	1.3451
24	1.3695	1.3929	1.4231
28	1.3924	1.4316	1.4826

The increase of k_∞ with coolant voiding has already been reported [10]. The importance of neutron absorption and slowing-down in light water coolant explain this behavior. Also, note that our results presented in Table 7 are consistent with those reported in the literature [13], i.e. k_∞ increases with lattice pitch. This behavior is typical of undermoderated nuclear reactors. In our case, the k_∞ are quite high because we are using a different CANFLEX bundle design and a higher fuel enrichment (the CANDU-SCWR lattice cell is still in evolution).

Figure 2 presents the average neutron flux in the moderator and in the fuel regions and the neutron absorption rate in the fuel region as a function of neutron energy for different lattice

pitches in the case of the lattice cell C3. Here, only the case of the lattice cell C3 is presented because C3 is the lattice cell the most affected by the lattice pitch. As it will be explained later, the lattice pitch affects the lattice cells C1 and C2 in the same way as the lattice cell C3, but in a less significant manner. The staircase shape of the curves reflects the multigroup calculation.

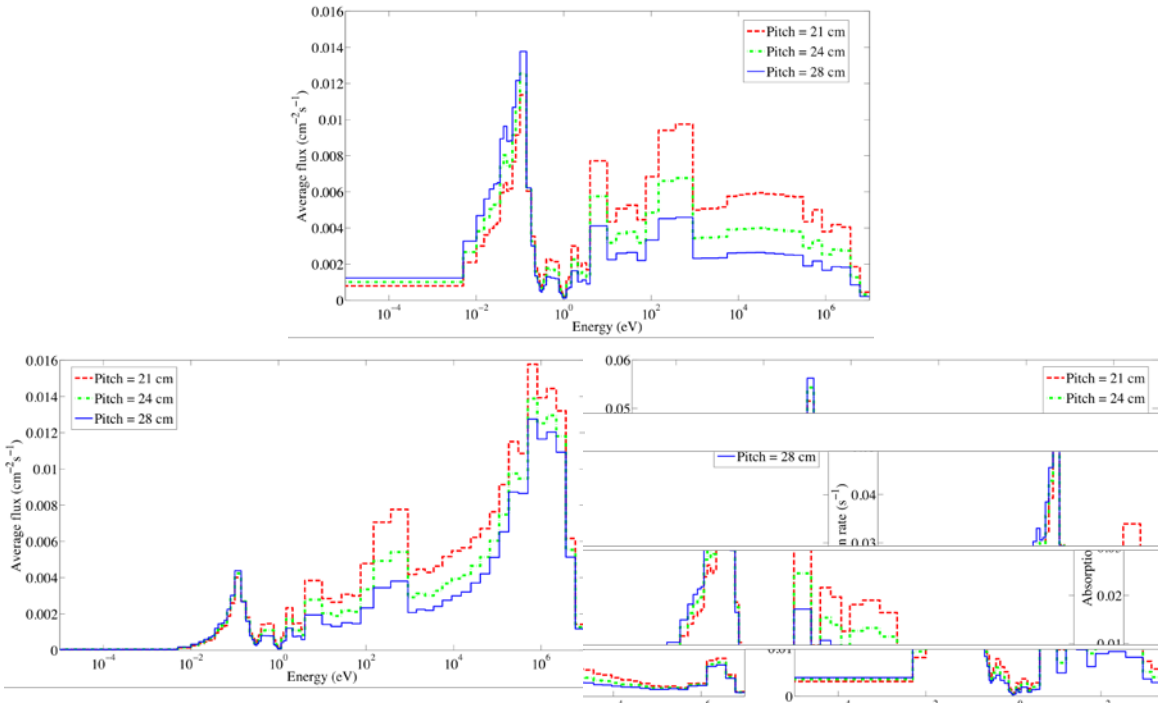

Figure 2 Average neutron flux in the moderator (a) and in the fuel (b) regions and neutron absorption rate in the fuel region (c) for lattice cell C3

The lattice pitch determines the volume of heavy water between the fuel bundles and thus, it has a direct effect on the average neutron flux in the moderator region. The thermalization of neutrons increases with the lattice pitch. As shown in Figure 2a, the flux decreases significantly with the lattice pitch in the fast ($E \geq 100$ keV) and epithermal (0.625 eV $\leq E <$ 100 keV) energy domains and increases with the lattice pitch in the thermal (E < 0.625 eV) energy domain.

As shown in Figure 2b, the same behavior is observed for the average neutron flux in the fuel region. The neutron absorption rate in the fuel region decreases significantly with the lattice pitch in the epithermal energy domain (see Figure 2c). These losses are mainly due to radiative captures in ^{238}U resonances. We can also use the flux to get an approximation for k_∞

$$k_\infty \equiv \frac{\nu R_f}{R_a} = \frac{1}{R_a} \tag{1}$$

where νR_f, is normalize to 1 and $R_a = VN\phi\sigma_a$. Here ν is the average number of neutrons produced per fission, R_f is the fission reaction rate, R_a is the neutron absorption rate, V is the volume of the region considered, N is the number density of nucleus in the material, ϕ is the average neutron flux in the region considered and σ_a is the absorption microscopic cross section.

According to the equation 1, the decrease in neutron absorption rate causes k_∞ to increase as shown in Table 7. In other words, the increase of the lattice pitch allows more fast neutrons to escape radiative captures in ^{238}U resonances before reaching a second fuel element (^{235}U). This is the main effect of the lattice pitch.

We have observed that the variation of the neutron absorption rate due to the lattice pitch in the coolant region is about 100 times smaller than that in the fuel region. We have also observed that the variation of the neutron absorption rate due to the lattice pitch in the moderator region is negligible.

Finally, the effect of the lattice pitch is more important in the case of the lattice cell C3 than in the case of the lattice cell C1 because the lattice cell C1 undergoes an additional thermalization due to the importance of neutron slowing-down in light water coolant [10]. The coolant density in the lattice cell C1 is about 8 times higher than the coolant density in the lattice cell C3.

3. Description of the CANDU-SCWR assembly model

Because the lattice pitch of the CANDU-SCWR is relatively small (between 20 cm and 21 cm [3]) and the thermodynamic conditions vary widely from the reactor inlet to the reactor outlet, there is a strong coupling between neighboring cells. It has been demonstrated that the use of multicell models for main flux calculation is necessary to optimize the safety characteristics of the CANDU-SCWR with the DRAGON code [10]. Here again, a simplified geometry can be used for resonance self-shielding calculation.

3.1 Assembly for main flux calculation

The 2x2 assembly in checkerboard pattern considered here contains two different cell types, as shown in Figure 3, in order to take into account of the bi-directional flow of the coolant [10]. Isotropic periodic (translation) boundary conditions have been applied on all the external surfaces of the assembly in order to simulate an infinite checkerboard pattern. The local properties of the lattice cells C1 and C3 are described in Table 6.

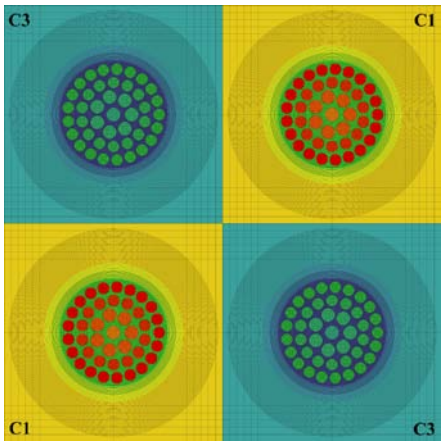

Figure 3 CANDU-SCWR 2x2 assembly in checkerboard pattern for main flux calculation

3.2 Geometry for resonance self-shielding calculation in assembly simulation

To determine the most appropriate geometry for resonance self-shielding calculation in the case of assembly simulation, we have developed five different models based on the following parameters:

- Geometry: It is possible to perform the resonance self-shielding calculation cell by cell (1x1) or by assembly (2x2). In the case of the calculation cell by cell, the resonance self-shielding calculation is achieved in two steps with a single lattice (as described in section 2.1.2): a first calculation is realized with the local properties of C1 followed by a second calculation realized with the local properties of C3. These two calculations are completely independent of each other. In the case of the calculation by assembly, the resonance self-shielding calculation is achieved in a single step using directly the 2x2 assembly presented in Figure 3, but without the spatial mesh discretization.

- Number of resonant regions: Isotopes with resonant cross sections, such as ^{235}U, ^{236}U, ^{238}U and ^{239}Pu, are concentrated in the fuel pins. In our model, all the fuel pins in the lattice cell are associated with the same region. Thus, in the case of the calculation cell by cell there is only one resonant region containing the 43 fuel pins. In the case of the calculation by assembly, there is two possibilities: 1) 1 resonant region containing the 172 fuel pins of the assembly or 2) 2 resonant regions containing the 86 fuel pins of the two lattice cells C1 in the first region and the 86 fuel pins of the two lattice cells C3 in the second region.

- Self-shielding correction options in the `SHI:` module of DRAGON: The option named `LEVE 0` corresponds to the original Stamm'ler model, the option named `LEVE 1` corresponds to the original Stamm'ler model with Nordheim approximation and the option named `LEVE 2` corresponds to the Stamm'ler model with Nordheim approximation and Riemann integration method [14].

From these parameters, five different models have been developed for the resonance self-shielding calculation. For each of them, k_∞ has been evaluated as presented in Table 8. The total computational time includes the analysis of the geometries, the resonance self-shielding and the main flux calculations. Here, a lattice pitch equals to 21 cm has been used for each lattice cell in 1x1 and 2x2 geometries.

Table 7 DRAGON k_∞ for different models of resonance self-shielding calculation

Model	Geometry	Number of resonant regions	Correction option	k_∞	Total computational time (min)
A	1x1 (C1) 1x1 (C3)	1	`LEVE 0`	1.3510	745
B	2x2	1	`LEVE 0`	1.3521	743
C	2x2	2	`LEVE 0`	1.3510	750
D	2x2	2	`LEVE 1`	1.3494	758
E	2x2	2	`LEVE 2`	1.3488	762

The 2x2 geometry takes into account of interactions between neighboring cells of the CANDU-SCWR in a better way than the 1x1 geometry. Thus, models C, D and E are certainly more appropriate. Although the model B uses the 2x2 geometry, the use of only 1 resonant region for all the assembly is a very rough approximation. This means that the

resonant region in C1 will share the same fine flux as the resonant region in C3. This is certainly not realistic because the local properties vary greatly between C1 and C3.

The model E is the ideal model since it uses the correction option LEVE 2 which leads to the most accurate results. However, this model requires considerable computing time and may not be adequate for 3-D and in-core depletion simulations. To improve the performance of our simulation, it is preferable to choose a simpler model. Model C for example, which uses the original Stamm'ler model to perform the resonance self-shielding calculation, could be a good candidate. There is only a difference of about 2.2 mk between the k_∞ of models C and E. An error of this order is not very significant, as it has already been mentioned. As one can see in Table 8, the model C leads to the same result as the model A. From the computational time point of view, it is advantageous to use the model A.

Finally, considering the total computational time (752 minutes on average), the computational time saved in this way may seem negligible (about 17 minutes between models A and E). However, this will result in an important difference (in hours) for 3-D and in-core depletion simulations.

4. Conclusion

In this study, the geometries used for resonance self-shielding calculation has been modeled in the DRAGON code. In the case of single lattice simulation, it has been shown that, unlike the geometry used for main flux calculation, the geometry used for resonance self-shielding calculation does not require a very fine spatial mesh discretization. In the case of 2x2 assembly simulations, we have chosen the simplest model that makes the best compromise between computational time and accuracy of results. This model consists in performing the resonance self-shielding calculation cell by cell rather than by assembly as it is done for the main flux calculation. Finally, from single lattice simulations, we have observed that the infinite multiplication constant increases with the lattice pitch. By analyzing neutron spectra and reaction rates obtained for different lattice pitches, we have observed that the increase of the lattice pitch reduces significantly the radiative captures in ^{238}U resonances.

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