MODELING OF A 3-D SCWR UNIT CELL

G. Harrisson and G. Marleau
Institut de génie nucléaire, École Polytechnique de Montréal
C.P. 6079, succ. Centre-ville
Montréal, Québec, Canada, H3C 3A7

Abstract

This paper presents the modeling of a 3-D Supercritical Water-Cooled Reactor unit cell. The pre-homogenization of the geometries allows us to reduce the size of the problem without affecting significantly the results of lattice cell calculations. The differences observed between the results of 2-D and 3-D calculations are explained by the isotropic reflective boundary conditions associated with the *Z* surfaces in the 3-D case. The lattice code DRAGON, which has the ability to solve the 3-D neutron transport equation, has been used in this study.

1. Introduction

From the neutronic perspective, the nuclear designer typically has the freedom to adjust any parameters that relate to the design of the lattice such as fuel enrichment, burnable poisons distribution and lattice pitch. To optimize the lattice design, several lattice cell calculations must be performed in order to evaluate the impact of these parameters on the reactivity coefficients and on the exit burnup for example. Lattice cell calculations are usually performed on a 2-D unit cell and with local conditions, such as coolant temperature and coolant density, that represent the average core conditions or the average conditions in the region of the core that produces the highest power.

As its name suggests, the Supercritical Water-Cooled Reactor (SCWR) operates at temperatures and pressures above the thermodynamic critical point of water (373.95 °C and 22.064 MPa). Figure 1 shows the significant variation in temperature and density of the coolant (light water) along a fuel channel of the pressure tube SCWR.

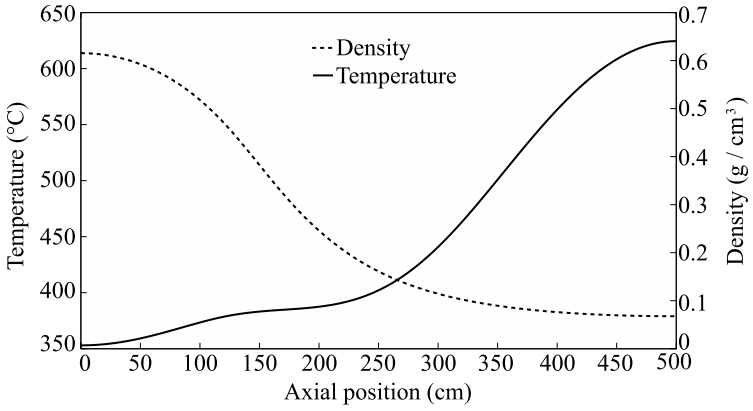


Figure 1 Coolant properties along a pressure tube SCWR fuel channel

For the pressure tube SCWR, it was observed that the exit burnup and the coolant void reactivity (CVR) vary depending on the axial position, i.e. depending on the set of local conditions found along the fuel channel [1]. Thus, it is not obvious which local conditions must be used to optimize the lattice design of the pressure tube SCWR. This requires a further study in which we will have to determine the neutronic properties of a 3-D fuel channel that takes into account the axial distribution of local conditions.

In this paper, we focus on the modeling of a 3D unit cell (L x L x L where L is the lattice pitch), which is a sub-element of the 3D fuel channel. To begin, Section 2 presents the unit cell used in this study. Then, in Section 3 we discuss the modeling of the unit cell in 2D and 3D. This section also assesses the benefits of using a pre-homogenization for the geometries used in these two models. Finally, in Section 4 we present some simulation results. In particular, the different models developed are compared. All calculations presented here were made with DRAGON 3.6 [2] and with the "iaea" multigroup cross section library downloaded from the WLUP 's web site [3].

2. Unit cell description

Neglecting all reactivity devices, the nuclear reactor core comprises an array of unit cells. As depicted in figure 2, the unit cell used in our lattice calculations is a high efficiency fuel channel [4], a 54 elements fuel bundle and a central coolant pin [5, 6].

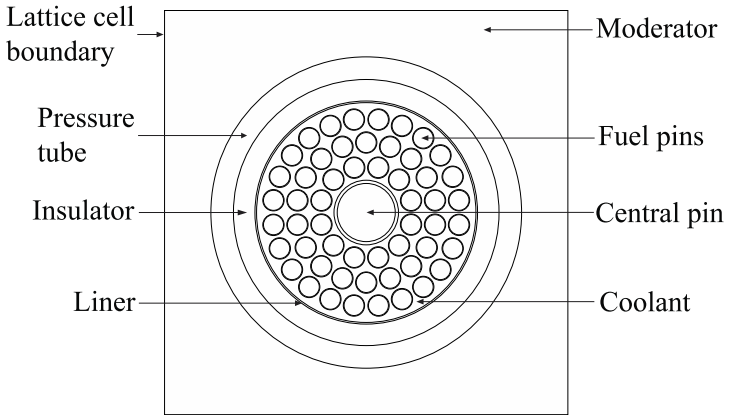


Figure 2 Unit cell as defined in DRAGON

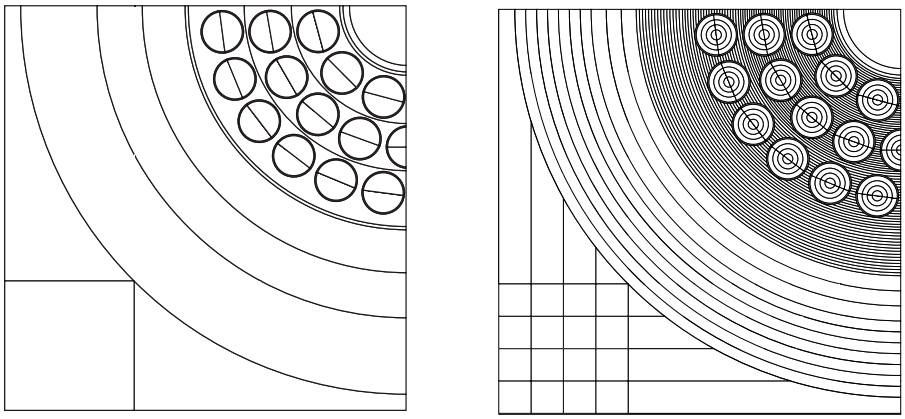
The high efficiency fuel channel is composed (from the inside to the outside) of a perforated stainless steel liner, insulating segments of zirconia and a pressure tube made of a zirconium alloy. Note that the openings through the liner and insulator are not explicitly illustrated in figure 2 since that type of geometry cannot be modeled in DRAGON. However, in order to take their effect into account, the liner and insulator mixtures are diluted with water (70 % of light water). The fuel bundle comprises a 3 rings array composed of respectively 12, 18 and 24 fuel rods, with the fuel being a mixture of thorium and plutonium from spent fuel recycling. The central pin is filled with coolant. Both the fuel rods and the center pin are covered by a sheath of stainless steel. The moderator uses heavy water, and the lattice pitch is set at 25 cm.

3. Unit cell modeling

The unit cell was modeled in 2-D and 3-D. The resulting geometries were pre-homogenized in order to reduce the size of the problems to be solved numerically.

3.1 2-D unit cell modeling

Modeling of the unit cell in 2-D requires to optimize the spatial mesh discretization and the tracking parameters of the geometries used for the main flux and the resonance self-shielding calculations. The following figure illustrates the resulting geometries, obtained after pre-homogenization. Isotropic reflective boundary conditions were applied on all outer surfaces of the geometries.



a b

Figure 3 Geometries used for the resonance self-shielding (a) and the main flux (b) calculations

Before applying the automatic spatial mesh discretization options of DRAGON, each fuel pin was divided in two symmetric regions in order to allow the definition of two different mixtures per pin. A different fuel mixture is associated with each half-pin (present on the same side of a ring) in order to obtain a total of 6 different fuel mixtures. This meshing is motivated by the fact that each half pin (facing or opposite the centre of the cell) is subject to a different environment and therefore to a different neutron flux. This can be justified as follow:

- The fuel pins in the inner ring are affected differently by the central coolant pin and the second ring of fuel pins;
- The central ring is in an environment where it sees fuel pins both towards the center of the cell and outwards;
- The outer half of the fuel pins in the outer ring sees mainly neutrons coming from the moderator while the inner half sees neutrons produced from the fuel pins in the central ring.

The central pin does not require such a meshing because it is in an axisymmetric position.

A different resonant region is also associated with each fuel mixtures. As a result, the resonance self-shielding calculation will decouple the different resonant regions using a correction option

corresponding to the original Stamm'ler model with Nordheim approximation (option LEVE 1 in the SHI: module) [7].

In our calculations, the collision probability method was used to solve the neutron transport equation. Thus, the spatial mesh discretization (either radial or Cartesian) of the geometry used for the main flux calculation must be fine enough to ensure the validity of the collision probability method that requires the sources to be constant in all the regions of the geometry. The spatial mesh discretization of this geometry was optimised by studying the infinite multiplication factor (k_∞) and some macroscopic cross sections ($\nu\Sigma_f$, Σ_a, Σ_s and Σ) based on the number of sub-regions in each region [8, 9]. Table 1 shows the optimized spatial mesh discretization of the geometry used for the main flux calculation. Here convergence was assumed when differences of less than 0.1 mk for k_∞ and 0.1 % for all two groups cell averaged cross sections were observed.

Table 1 Optimized spatial mesh discretization in the *x-y* plane

	Geometry for resonance self-shielding calculation	**Geometry for main flux calculation**
Region	**Optimized radial mesh discretization (sub-regions)**	
Central pin	1	1
Fuel pins	1	4
Sheaths	1	1
Coolant	4	64
Liner	1	1
Insulator	1	14
Pressure tube	1	3
Moderator	1	7
	Optimized Cartesian mesh discretization (squares per corner)	
Corners	1	16

The optimization of the spatial mesh discretization has been performed for three sets of local conditions, i.e. those found at z = 25 cm, z = 175 cm and z = 475 cm. As illustrated in figure 1, the coolant density at these axial positions is near its maximum, average and minimum value. The results show that the optimized spatial mesh discretization does not depend on local conditions.

Furthermore, as shown in table 1, it was found that a coarse spatial mesh discretization of the geometry is acceptable for the resonance self-shielding calculation. This conclusion results from a comparison of the neutronic properties of the unit cell obtained with the fine against those obtained with the coarse spatial mesh discretization. The resulting differences show a negligible effect on two groups cell averaged cross sections (less than 0.07 %) and a small effect on k_∞ (less than 0.34 mk).

The density of the integration lines (*dens* in lines per cm) must be maximised in order to reach each region and surface of the geometry as often as possible. Similarly, the number of integration angles (*nangl*), which can take any value for 2-D geometries with isotropic reflective

boundary conditions, must be maximised in order to be able to simulate as many neutron trajectories as possible. The selected *dens* and *nangl* limit the numerical integration errors on both volumes and surfaces at 1.0 % when compared with the exact values. The following table shows the optimized tracking parameters.

Table 2 Optimized tracking parameters for the 2-D unit cell

	Geometry for resonance self-shielding calculation	**Geometry for main flux calculation**
dens (lines/cm)	20.0	35.0
nangl (equidistant angles on [0, π/2])	20	20

3.2 3-D unit cell modeling

The 3-D unit cell model requires a 3-D geometry for the main flux calculation and, a priori, another for the resonance self-shielding calculation. These geometries were created by extending the 2-D geometries described in the previous section on a distance of 25 cm in the axial direction, i.e. along the *z*-axis. Isotropic reflective boundary conditions were applied on all outer surfaces of the geometries.

The study of the neutronic properties as a function of the mesh splitting of the geometry along the *z*-axis showed that the 3-D unit cell does not require an additional spatial mesh discretization. The differences between a fine (25 slices of 1 cm thick) and a coarse (1 slice of 25 cm thick) Cartesian mesh discretization along the *z*-axis are negligible (0.05 mk for k_∞ and a maximum of 0.09 % for two groups cell averaged cross sections). This would be expected for a totally reflected cell with specular boundary conditions (mirror reflections) at the faces normal to the *z*-axis. It also proved to be true in our case where white boundary conditions are selected (isotropic reflection).

For 3-D geometries, the tracking parameters are determined by the density of the integration lines (*dens* in lines per cm^2) and by the angular quadrature order (*N*). In the case of an equal weight EQ_N quadrature, the value of *N* is limited to 2, 4, 8, 10, 12, 14 or 16 [10]. For a quadrature of order *N*, a total of $4N(N + 2)/8$ angular directions are selected in the upper half-sphere. The selected *dens* and *N* limit the numerical integration errors on volumes at 1.0 % and on surfaces at 10.0 % when compared with the exact values. Table 3 shows the optimized tracking parameters for the geometries in 3-D.

Table 3 Optimized tracking parameters for the 3-D unit cell

	Geometry for resonance self-shielding calculation	**Geometry for main flux calculation**
dens (lines/cm^2)	100.0	200.0
N (EQ_N quadrature)	8	10

3.3 Pre-homogenization of the geometries

In our case, the pre-homogenization of the geometries allows to:

- Remove the Cartesian mesh discretization which is superimposed on the radial mesh discretization in the moderator and the pressure tube regions.
- Take advantage of the ¼ symmetry of the unit cell (a first reflection axis parallel to the *y*-axis and a second parallel to the *x*-axis, both axes being located at the center of the unit cell).

The action of pre-homogenizing consists of combining two or more regions (or surfaces) into one region (or surface) later referred to as combined. This action requires that all regions belonging to the combined region share the same flux. The pre-homogenization of the geometries allows us to reduce the size of the problems to be solved by reducing the number of unknowns in the main flux calculation.

In our case, pre-homogenization is done after creating the tracking data structure containing the volume of regions and the area of surfaces of the geometry, but before creating the sequential binary tracking file containing the lengths of the integration lines. Thus, pre-homogenization modifies only the data in the tracking data structure. The following list shows the calculation procedure followed in DRAGON:

- Creating a local multigroup cross section library with the `LIB:` module;
- Creating a geometry with the `GEO:` module;
- Creating the tracking data structure with the `NXT:` module (using the `NOTR` option to avoid tracking the geometry);
- Modifying the tracking data structure by pre-homogenizing the geometry with the `MRG:` module;
- Creating the sequential binary tracking file and modifying the tracking data structure with the `NXT:` module, while taking into account the combined regions and surfaces;
- Calculating the resonance self-shielding with the `SHI:` module;
- Calculating the fluxes with the `ASM:` module, followed by the `FLU:` module;
- Editing the results with the `EDI:` module.

Up to now, the `MRG:` module was used to pre-homogenize a geometry after being tracked with the `EXCELT:` module. However, the complexity of the geometries of this case of study cannot be tracked with the `EXCELT:` module for the following reasons:

- The fuel pins contain a Cartesian mesh discretization;
- The 2-D unit cell comprises both fuel pins and Cartesian mesh discretization;
- The 3-D unit cell comprises fuel pins.

Consequently, changes were made in some subroutines of DRAGON in order to allow the pre-homogenization of geometries after being tracked or analysed with the `NXT:` tracking module. Table 4 presents the effect of the pre-homogenization on our geometries.

Table 4 Impact of the pre-homogenization on the number of regions and surfaces comprised in the geometries

	Geometry for resonance self-shielding calculation	**Geometry for main flux calculation**
	2-D unit cell	
Without MRG:	38 regions and 12 surfaces	301 regions and 36 surfaces
With MRG:	25 regions and 4 surfaces	145 regions and 10 surfaces
	3-D unit cell	
Without MRG:	38 regions and 88 surfaces	301 regions and 638 surfaces
With MRG:	25 regions and 54 surfaces	145 regions and 300 surfaces

4. SIMULATION RESULTS

In the case of the 3-D unit cell, we have shown that it is possible to perform the resonance self-shielding calculation in 2-D (figure 3a), rather than in 3-D, without significantly affecting the results of lattice cell calculations. A difference of about 0.3 mk for k_∞ was observed between these two cases (at z = 175 cm). Note that the 3-D results presented in this section were obtained by performing the resonance self-shielding calculations in 2-D in order to simplify the problems to be solved.

Table 5 shows the value of k_∞ obtained from the models developed and from three sets of local conditions.

Table 5 DRAGON k_∞

	2-D unit cell			**3-D unit cell**		
Axial position (cm)	**25**	**175**	**475**	**25**	**175**	**475**
Without MRG:	1.18029	1.18273	1.16262	1.17933	1.18237	1.16550
With MRG:	1.18031	1.18275	1.16262	1.17935	1.18239	1.16550

According to this table, there is at most a difference of 0.02 mk between the models with and without the pre-homogenization of the geometries. This small difference indicates that the our simplification do not affect the calculation results.

Also according to table 5, there is at most, for an equivalent angular quadrature, a difference of 2.88 mk (at z = 475 cm) between the 2-D and 3-D models. In the 2-D case, the unit cell, defined in the x-y plane, extends to infinity along the z-axis while in the 3-D case, the unit cell domain along the z-axis is limited. Thus, the absence of boundary conditions in the z direction for the 2-D case (effectively an infinite cell) and the presence of isotropic reflective boundary conditions associated with the Z surfaces in the 3-D case are the causes of this difference.

5. CONCLUSION

In this study, a 3-D unit cell was modeled for the pressure tube SCWR. In our model, in order to eliminate the superposition of the different spatial mesh discretization and to take advantage of the unit cell symmetry, changes have been made in some DRAGON subroutines. These changes allow us to pre-homogenize, with the `MRG:` module, geometries tracked or analyzed with the `NXT:` module. A maximum difference of 0.02 mk between the original and the simplified models was observed. In addition, for an equivalent angular quadrature and for the same sets of local conditions, a maximum difference of 2.88 mk was observed between 2-D and 3-D calculations. The isotropic reflective boundary conditions applied on *Z* surfaces in the 3-D case give rise to this difference.

6. ACKNOWLEDGEMENTS

This work was supported in part by the NSERC/NRCan/AECL Generation IV Energy Technologies Program, by the Fonds québécois de la recherche sur la nature et les technologies and by the Canadian Nuclear Society.

We would like to thanks Bronwyn Hyland and Jeremy Pencer for this research idea and for the fruitful discussions held since the summer of 2010 on this topic.

7. REFERENCES

[1] R.G. Dworschak, ‘‘The use of Response Surface Methodology (RSM) to scope Gen IV Super Critical Water Reactor (SCWR) thorium fuel cycle parameters’’, American Nuclear Society – 4th Topical Meeting on Advances in Nuclear Fuel Management, Hilton Head Island, South Carolina, USA, 2009, April 12-15, pp. 651-670.

[2] G. Marleau, A. Hébert and R. Roy, ‘‘A user guide for DRAGON 3.06’’, École Polytechnique de Montréal, Montréal, Québec, Canada, Technical report IGE-174 Rev.7, 2008.

[3] NAPC Nuclear Data Section, ‘‘*WIMS-D Library Update Project*’’, 2005. [On line]. Available: www-nds.iaea.org/wimsd.

[4] C.K. Chow and H.F. Khartabil, ‘‘Conceptual Fuel Channel Designs for CANDU-SCWR’’, *Nuclear Engineering and Technology*, Vol. 40, Iss. 2, 2008, pp. 139-146.

[5] P.G. Boczar, W. Shen, J. Pencer, B. Hyland, P.S.W. Chan and R.G. Dworschak, ‘‘Reactor Physics Studies for a Pressure Tube Supercritical Water Reactor (PT-SCWR)’’, The 2nd Canada-China Joint Workshop on Supercritical Water-Cooled Reactors, Toronto, Ontario, Canada, 2010, April 25-28.

[6] M. Magill, J. Pencer, R. Pratt, W. Young, G.W.R. Edwards and B. Hyland, ‘‘Thorium Fuel Cycles in the CANDU Supercritical Water Reactor’’, The 5th International Symposium On Supercritical Water-Cooled Reactors, Vancouver, British Columbia, Canada, 2011, March 13-16.

[7] A. Hébert, ‘‘Revisiting the Stamm’ler self-shielding method’’, 25th Annual CNS Conference - Nuclear Energy: Meeting the Challenges, Toronto, Ontario, Canada, 2004, June 6-9, pp. 333-341.

[8] G. Harrisson and G. Marleau, ‘‘Models for safety analysis of the generation IV supercritical water-cooled reactor’’, The 2nd Canada-China Joint Workshop on Supercritical Water-Cooled Reactors, Toronto, Ontario, Canada, 2010, April 25-28.

[9] G. Harrisson and G. Marleau, ‘‘Models for resonance self-shielding calculation in neutronic analysis of the CANDU-SCWR fuel channel’’, 31st Annual CNS Conference - Atoms for Power, Health & the Environment, Montréal, Québec, Canada, 2010, May 24-27.

[10] B.G. Carlson, ‘‘Tables of equal weight quadrature EQ_N over the unit sphere’’, Los Alamos National Laboratory, Los Alamos, Report LA-4734, 1971.