# Optimization of the Fuel Assembly for the Canadian <u>Supercritical Water-cooled Reactor (SCWR)</u>

Corey French<sup>1</sup>, Dr. Hugues Bonin<sup>1</sup>, Dr. Paul Chan<sup>1</sup> <sup>1</sup> Department of Chemistry & Chemical Engineering, Royal Military College of Canada Corey.French@rmc.ca *M.A.Sc. Level Submission* 

#### Summary

A parametric optimization of the Canadian Supercritical Water-cooled Reactor (SCWR) lattice geometry and fresh fuel content is performed in this work. With the potential to improve core physics and performance, significant gains to operating and safety margins could be achieved through slight progressions. The fuel performance codes WIMS-AECL and SERPENT are used to calculate performance factors, and use them as inputs to an optimization algorithm.

## 1. Introduction: The Next Generation

The Canadian SCWR, or pressure tube (PT) SCWR, has been proposed as Canada's contribution to the Generation-IV International Forum (GIF). This cooperative international organisation, formed in 2001 by several countries, has in vision to investigate next-generation nuclear energy systems for sustainable energy [1]. In turn, the reactor concepts exhibit traits which contribute to the social, environmental and economic aspects of sustainable energy. The SCWR is a heavy-water moderated, light-water cooled reactor which operates at very high pressure and temperature in order to take advantage of the enhanced heat transfer properties of supercritical water. These enhanced properties result in a thermal efficiency of about 48% for the SCWR; quite an improvement over the 30-33% thermal efficiency for the conventional CANDU reactor[2]. Not only does this result in a better utilization of the fission energy, but also that for the SCWR only 52% of the energy is rejected to the environment. The reactor will be fueled with a thorium-based fuel with an initial slight enrichment of fissile material.

#### 2. Design: 78-Pin & 64-Pin Fuel Assemblies

There are two lattice designs that are currently under industry development: the 2D benchmark 78-element fuel assembly and the 64-element fuel assembly, which are shown in Figures 1 and 2. Both of the 5 metre long fuel assemblies for these lattices are inserted in High Efficiency reentrant Channels (HEC), consisting of zirconia-modified 310 stainless steel (SS) inner liner, porous zirconia (Zr) insulator and an excel PT which is in direct contact with the moderator. The fuel used in the assemblies are thoria(Th)-based, and expected to be enriched with recycled reactor grade plutonium (Pu). The central flow tube drives the coolant down from the inlet to the bottom of the assembly, and it recirculates up to the outlet via the sub-channel. Since the SCW environment is expected to be highly corrosive, a Zr-modifed 310 SS clad is to be used, despite the inferior neutronic properties of this material [3].

## 3. Methodology

#### 3.1 **Objective of Research and Benchmark**

Dedicated efforts in thermal hydraulics, fuel design and reactor physics are committed within the industry to refining the initial designs of this advanced reactor for its optimal performance in factors such as the burnup, the channel void reactivity (CVR), the critical heat flux (CHF), the linear element rating (LER), among others [4]. The objective of this work is to investigate the feasibility of applying a generic optimization technique to both fuel assembly designs for use in the Canadian SCWR. For the purpose of this investigation, the decision variables of the optimization problem are described below in Figures 1 and 2. These are the parameters that can be controlled within the model, and are ultimately the set of quantities needed to be determined to solve the optimization problem.



Figure 1: 78-Pin Fuel Assembly [5]

Figure 2: 64-Pin Fuel Assembly [6]

#### 3.2 **Optimisation Problem: Objective Function, Decision Variables and Constraints**

The decision variables are used to calculate an objective function, or Index of Performance (IP), that include Performance Factors (PF) such as the fuel discharge burnup, the surface heat flux (SHF), and the Radial Form Factor (RFF). The PF consist of physical computations of the respective lattice operational powers and temperatures, and give insight to the change in physical behaviour of the core. The burnup factor is a measure of the energy extracted from the primary nuclear fuel source, whose targeted value is a maximum. The remaining two factors have minimums as target values. The SHF is a measure of the rate of heat energy transfer through the clad of the fuel, and is dependent on the fuel centreline temperature. Conversely the RFF is the ratio of the pin with the highest rod power density (RPD) to the average pin RPD in a fuel assembly, and dictates the distribution of power in the fuel channel and subsequent lattices. These components that form the IP are ultimately optimized (typically minimized) using a steepest descent method such as the Gauss method, or with support from a conjugate gradient

method such as Hestene's method. The fuel assembly design is first structured into a mathematical reactor model for both pin assemblies, and a generic technique for solving an optimization problem is applied. Following the solution to the neutron transport equation computed from the fuel performance codes, the PF are used as inputs to the optimisation model algorithm. The purpose of the optimisation process is to use a numerical technique to evaluate the IP based on the sum of weighted squares of the PF;

$$IP = \sum_{i=1}^{m} \varphi_i^T \left( \vec{x}^{(k)} \right) \cdot \varphi_i \left( \vec{x}^{(k)} \right) = \underbrace{\left( w_1 \varphi_1 \right)}_{Burnup}^{-2} + \underbrace{\left( w_2 \varphi_2 \right)}_{SHF}^{2} + \underbrace{\left( w_3 \varphi_3 \right)}_{RFF}^{2}$$
(1)<sup>1</sup>

and to subsequently minimize the IP by calculating optimal values for the DV. In other words, based on a DV start point  $\bar{x}_0$ , there is an amount,  $\delta \bar{x}$ , by which we can vary the DV iteratively until convergence is obtained with the IP. This amount can be analytically represented as:

$$\delta \vec{x} = \left(J^{T(k)} J^{(k)}\right)^{-1} J^{T(k)} \left(-\vec{\varphi}^{(k)}\right)$$
(2)

where  $J_k$  represents the Jacobian  $m \ge n$  matrix  $\left(J_{m,n}^{(k)} = -\varphi_m'(x_n^{(k)})\right)$ ; an assembly of the partial derivatives of PF  $(\bar{\varphi}_m)$  taken with respect to the DV  $(\bar{x}_n)$  at iteration k. In this steepest descent method, taking the negative gradient of the PF with respect to the DV analytically chooses the direction in which the IP decreases most quickly towards the minimum. With consecutive iterations, convergence can be achieved with the IP straightforwardly by calculating the percent difference between successive iterations. The iterative procedure is terminated when the difference becomes less than a convergence criterion chosen by the analyst. The complete mathematical optimisation model with be housed within MATLAB. The compatible input and output files types of fuel performance codes to be used make for simple manipulation of data within MATLAB. The operator of the optimisation model also has control over the algorithm. At any point through the iterations, the user can stop the process and change the tolerance or step size in order to help convergence. This ensures accuracy of the model, consistency and ensures that constraints are respected throughout the algorithm process. At this point also, the user could also implement a different type of numerical technique such as a conjugate gradient method, to further aid with convergence.

#### 3.3 Fuel Performance Codes: WIMS-AECL & SERPENT

The benchmark problem geometries for both lattice designs are modelled with the deterministic code WIMS-AECL3.1.2.1 by the computational reactor physics branch at Atomic Energy of Canada Ltd (AECL) [7]. The WIMS-AECL models create the geometric lattices observed in

<sup>&</sup>lt;sup>1</sup> Typically in Canada, optimisation techniques search for a solution which is a minimum. Hence the algorithm searches for a minimum to the IP. Since burnup is to be maximized, a negative exponent is incorporated into the equation for its minimisation.

Figures 1 and 2, which represent a 2D axial slice along the fuel channel. In order to accurately model fluence, coolant temperature and density along the channel, five axial slice locations are used to model the likes of a fuel channel. These conditions for these axial positions can be observed in Table 1. Criticality and burnup calculations from WIMS models at these locations are used for code-to-code comparison with similar SERPENT models.

Table 1. Coolant Density & Temperature for Five Axia Positions along the SCWK Fuel Channel [8]							
Distance from	Coolant density	Coolant temp	Clad temp	Insulator temp	PT temp		
channel outlet (m)	(kg·m <sup>-</sup> )	(K)	(K)	(K)	(K)		
4.5	592.54	632.35	796.35	554.88	477.55		
3.5	382.46	656.30	808.30	570.83	485.51		
2.5	160.92	675.27	817.76	583.46	491.82		
1.5	89.49	774.05	867.04	649.25	524.65		
0.5	69.93	881.45	920.63	720.78	560.35		

Table 1: Coolant Density & Temperature for Five Axial Positions along the SCWR Fuel Channel<sup>2</sup> [8]

To obtain analytical perspective, a separate lattice code was developed in the probabilistic Monte Carlo code SERPENT v1.1.18 [9]. This code is generated to reproduce the benchmark methodology and geometry. The SERPENT models are used to compute the PF that are to be used in the optimization algorithm. Accordingly, the models are designed with a stand-alone burnup routine in addition to flux detectors on the surface of the fuel clad to compute the PF. It should be mentioned that all WIMS-AECL and SERPENT computations are performed using the Evaluated Nuclear Data File Beta-VII (ENDF/B-VII) neutron cross-section libraries.

# 4. **Preliminary results**

This section presents some fundamental results of the lattice codes on which the optimisation effort is based upon. In an initial code-to-code comparison the infinite multiplication factor,  $k_{\infty}$ , is calculated for the 78-pin lattice for the conditions described in Table 1. These results can be observed and compared in Table 2. For each criticality evaluation, WIMS-AECL and SERPENT both assume a freshly fueled channel that burns at full power until it becomes subcritical.

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Distance from	$\mathbf{k}_{\infty}$ - WIMS	$k_{\infty}$ - SERPENT	Relative difference			
channel outlet (m)	$(\pm 0.001)$	$(\pm 0.001)$	$[S-W]^3$ (mk)			
4.5	1.267	1.279	+ 12.1			
3.5	1.26657	1.275	+ 8.73			
2.5	1.26565	1.270	+ 4.12			
1.5	1.26458	1.259	- 5.7			
0.5	1.263	1.247	- 16.5			

Table 2: Infinite Multiplication Factor Comparison of WIMS & SERPENT (fresh fuel)

The fuel channel power is held constant in each trial. The results demonstrate that the initial SERPENT model agrees reasonably to the WIMS-AECL benchmark model. The criticality for

<sup>&</sup>lt;sup>2</sup> Table 1 represents conditions for the 78-element 2D benchmark design only. Similar, although pending, conditions for the 64element benchmark have yet to be released by AECL. These will be incorporated into the work upon receiving.

<sup>&</sup>lt;sup>3</sup> [S-W] =  $k_{\infty}$ (SERPENT) -  $k_{\infty}$ (WIMS)

both, as expected, increases as the position along the fuel channel approaches the outlet condition, that is, increased temperatures and pressures. The average percent difference in milli-k (mk) is  $\pm$  9.42 mk.

# 5. Discussion and Conclusions

This work is in its first 6 months of realization. The principal objective of this thesis considers the systematic application of numerical techniques for solving an optimization problem such as outlined in this paper. Preliminary results indicate that initial infinite multiplication factors calculated between WIMS-AECL and SERPENT agree well for the 78-pin arrangement, and similar trends are expected to be observed with the 64-pin lattice. Further code-to-code comparison can be investigated through implementation of the burnup routine in SERPENT for additional code support. The impact of the model is to offer a generic tool for lattice and assembly geometry optimisation. It could ultimately be used as a supplementary tool in industry and regulation used in operations, trip and safety margin analysis.

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