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OPTIMIZATION OF THE FUEL ASSEMBLY FOR THE CANADIAN SUPERCRITICAL WATER-COOLED REACTOR (SCWR)

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ABSTRACT – An approach to develop a parametric optimization tool to support the Canadian Supercritical Water-cooled Reactor (SCWR) fuel design is presented in this work. The 2D benchmark lattices for 78-pin and 64-pin fuel assemblies are used as the initial models from which fuel performance and subsequent optimization stem from. A tandem optimization procedure is integrated which employs the steepest descent method. The physics codes WIMS-AECL, MCNP6 and SERPENT are used to calculate and verify select performance factors. The results are used as inputs to an optimization algorithm that yield optimal fresh fuel isotopic composition and lattice geometry. Preliminary results on verifications of infinite lattice reactivity are demonstrated in this paper.

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) for next-generation energy systems. This cooperative international organization, formed in 2001 by several countries, has as mandate to investigate next-generation nuclear energy systems envisioned 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 light water in the supercritical regime. 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 thermal energy is rejected to the environment. The reactor will use an advanced fuel cycle which is thorium-based. The fertile fuel source will be driven with an initial amount of fissile plutonium to sustain the fuel cycle. From a design perspective, there is potential to improve lattice and core physics, which translates into improved operational performance and control. From a safety analysis perspective, further performance and control translate into significant gains to margin that are achieved through slight progressions.

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

There are two lattice designs that are currently under industry development: the 2D benchmark lattices for the 78-element fuel bundle and the 64-element fuel assembly, which are presented in Figures 1 and 2. The former design comprises of half-meter bundles; ten of which are present in a

fuel channel. The latter consists of one 5 meter fuel assembly. Both of the 5 meter long fuel assemblies for these lattices are inserted in High Efficiency re-entrant 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 is thorium (Th)-based, and expected to use recycled reactor grade plutonium (Pu) as the driving source of fissile material. In the 78-pin design, the center-pin consists of a solid Yttrium-stabilized Zr rod, which does not contribute to the fission power, but rather to decrease Coolant Void Reactivity (CVR). Inversely, the 64-pin design comprises a central flow tube that 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].

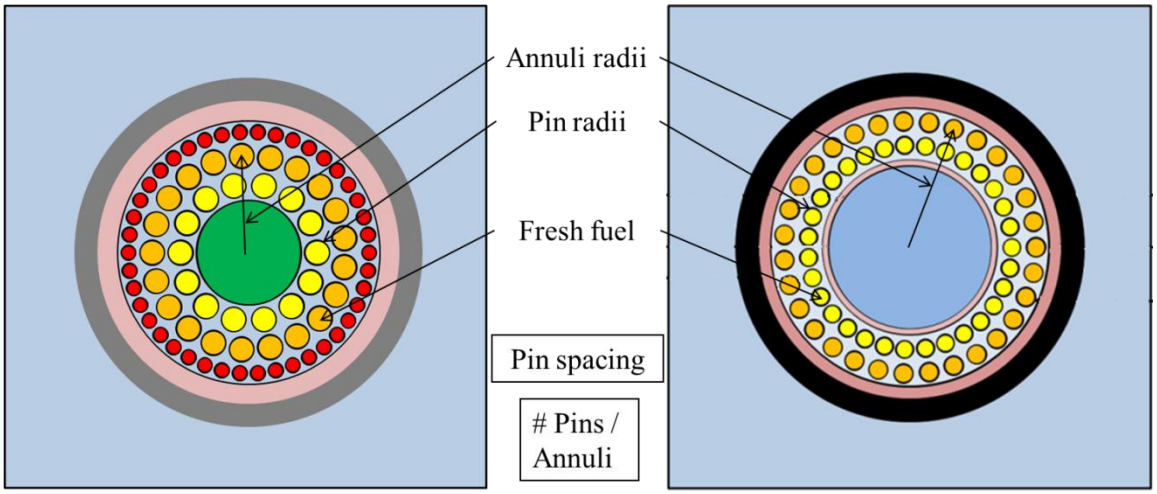

Figure 1: 78-Pin Fuel Assembly [4] **Figure 2: 64-Pin Fuel Assembly [5]**

3. Methodology

3.1 Objective of Research

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 CVR, the critical heat flux (CHF), the linear element rating (LER), among others [6]. The objective of this work is to develop a generic optimization toolset operable on a single computer platform, and subsequently to investigate the feasibility of applying this technique to both fuel designs for use in the Canadian SCWR. For the purpose of this investigation, the decision variables of the optimization problem are outlined below in Table 1. These are the parameters that can be controlled and modified within the model, and are ultimately the set of variables computed in the solution to the optimization problem algorithm.

Table 1: The Decision Variables for the Optimization Problem

Decision Variable		78-Pin Bundle	64-Pin Assembly
Fuel Composition	Plutonium Content	$\chi_1^{78}, \chi_2^{78}, \chi_3^{78}$	χ_1^{64}, χ_2^{64}
Geometry	Fuel Rod Radius	$r_{cp}^{78}, r_1^{78}, r_2^{78}, r_3^{78}$	$r_{R.C.}^{64}, r_1^{64}, r_2^{64}$
	Annulus Radius	$R_1^{78}, R_2^{78}, R_3^{78}$	R_1^{64}, R_2^{64}
	# Rods per Annulus	$N_1^{78}, N_2^{78}, N_3^{78}$	N_1^{64}, N_2^{64}

3.2 Optimization Problem: Objective Function, Performance Factors and Constraints

The aforementioned decision variables are used to calculate an objective function, or Index of Performance (IP), which include three key Performance Factors (PF); namely 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, giving insight to the change in physical behaviour of the core over time. 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 centerline temperature. The current design requirement is that sheath temperature is limited to 1000K. Conversely the RFF is the ratio of the pin with the highest rod power density (RPD) to the average RPD in a fuel bundle or assembly, and dictates the distribution of power in the fuel channel and subsequent lattices. It is essential for a balance of power, and inherent control, to have all fuel elements producing near-average power.

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 other methods such as conjugate gradient method or genetic algorithm. 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 optimization model algorithm. The purpose of the optimization process is to use a numerical technique to evaluate the IP based on the sum of weighted squares of the PF;

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

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

[1] 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.

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

where J_k represents the Jacobian m x n matrix $\left(J_{m,n}^{(k)} = -\varphi_m{}'\left(x_n^{(k)} \right) \right)$; an assembly of the partial derivatives of PF $\left(\vec{\varphi}_m \right)$ taken with respect to the DV $\left(\vec{x}_n \right)$ 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. A flow chart of this methodology is presented as Figure 3.

The complete mathematical optimization 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 and subsequent processing within MATLAB. The user of the optimization model also has control over the algorithm. At any point throughout 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 lattice geometries for both fuel designs are modeled 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 Figures 1 and 2, which represent a 2D axial slice along the fuel channel. In order to accurately model the fluence, the coolant temperature and the density along the fuel channel, five axial slice locations are used to model the likes of a fuel channel. The conditions for these axial positions can be observed in Table 2. Criticality and burnup calculations are performed with the WIMS models at these locations, and the results are used for code-to-code comparison with similar stochastic MCNP6 and SERPENT models.

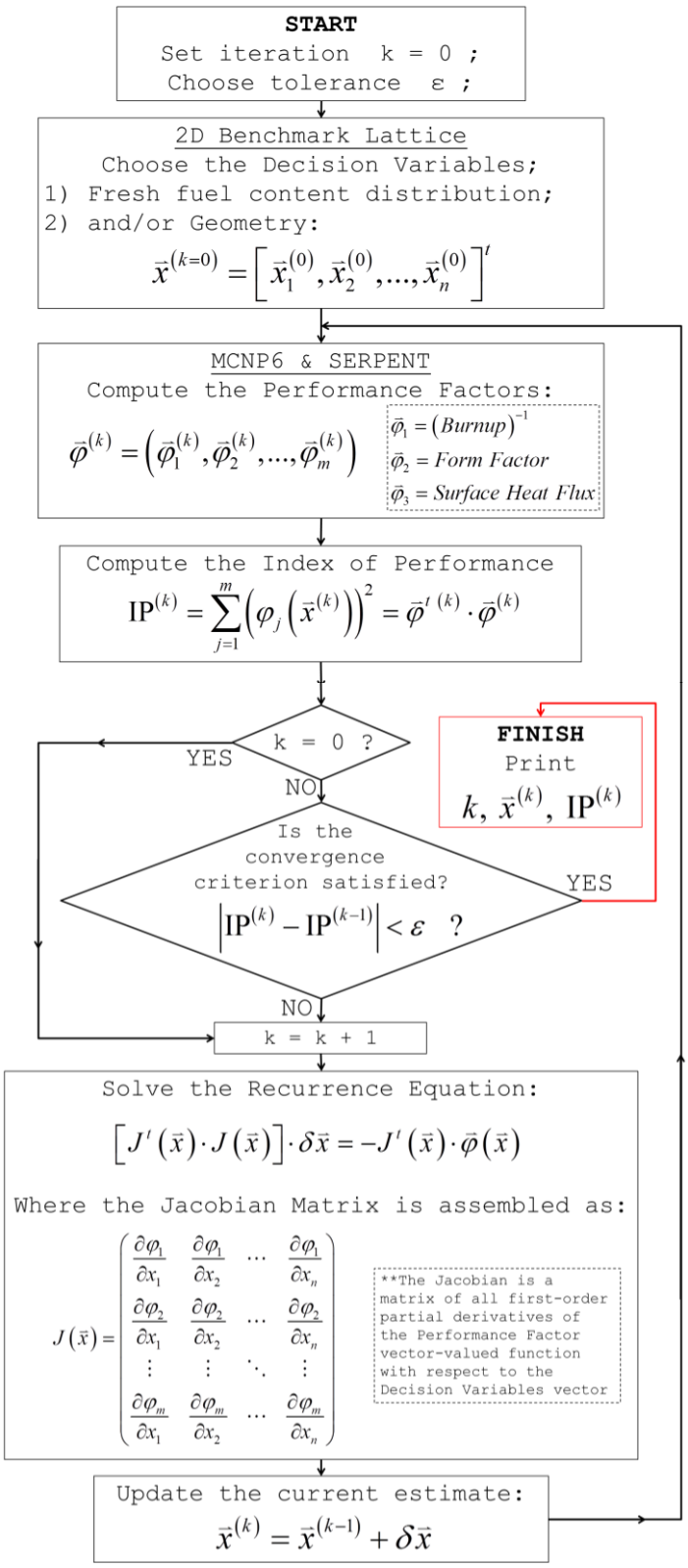

Figure 3: Optimization Methodology Flow Chart Using the Gauss Steepest Descent Method

Table 2: Coolant Density & Temperature for Five Axial Positions along the SCWR Fuel Channel for the 78-Pin Lattice[2] [8]

Distance from channel outlet (m)	Coolant Density ($kg \cdot m^{-3}$)	Coolant Temp. (K)	Clad Temp. (K)	Insulator Temp. (K)	PT Temp. (K)
0.5	69.93	881.45	920.63	720.78	560.35
1.5	89.49	774.05	867.04	649.25	524.65
2.5	160.92	675.27	817.76	583.46	491.82
3.5	382.46	656.30	808.30	570.83	485.51
4.5	592.54	632.35	796.35	554.88	477.55

To obtain analytical perspective, a separate lattice code was developed in the probabilistic Monte Carlo code SERPENT v1.1.18 and the Los Alamos code MCNP6 [9,10]. Both codes are 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 optimization effort will be based upon. In an initial code-to-code verification of the infinite multiplication factor, k_∞, is calculated for the 78-pin lattice for the conditions described in Table 2. The results can be observed and compared in Table 3. For each criticality evaluation, WIMS-AECL and SERPENT both assume a freshly fueled channel that burns at full power until it becomes subcritical.

Table 3: Infinite Multiplication Factor Comparison of WIMS & SERPENT (for fresh fuel)

Distance from Channel Outlet (m)	k_∞ - WIMS (± 0.001)	k_∞ - SERPENT (± 0.001)	Relative Difference [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

[2] Table 1 represents conditions for the 78-element 2D benchmark design only. Similar, although pending, conditions for the 64-element benchmark have yet to be released by AECL. These will be incorporated into the work upon receipt.
[3] [S-W] = k_∞(SERPENT) - k_∞(WIMS)

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 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 ± 9.42 mk. There is one emergent trend that can be gathered from these results, in that the criticality computed by SERPENT at the Beginning of Channel (BOC) is relatively lower than the benchmark WIMS-AECL case, compared to the End of Channel (EOC), where the SERPENT criticality is relatively higher than the reference. From the Relative Difference column of Table 3, it can be visualized that in the progression from BOC to EOC, the SERPENT k_∞ begins slightly below the WIMS value, and increases along the channel until it 'crosses' the WIMS profile near the center of the channel, continuing to increase until the EOC where it is slightly higher than the WIMS value.

Although the result is not ideal, it is important to note that the accuracy of the model is not of utmost importance in the entire scope of the work. It is important that the relation between models is well-known, which can be demonstrated. As the models are refined and the optimization routines are implemented, it is likely that the performance and design of the models will only improve. Therefore the improved result at a later iteration will always maintain the ability for comparison to an earlier performance of the model.

5. Discussion and Conclusions

An immediate concern that arises is due to the difference in criticality trends between SERPENT and WIMS-AECL. There are many potential root causes, inherent in both codes that are culprits of these effects. The first potential cause is the choice and difference of which nuclear data libraries are used in which codes. Since it was stressed that both codes use the ENDF/B-VII cross-section library, it is unlikely that this is the causation. However, there is a difference in how each code treats resonance self-shielding and temperature-dependent Doppler broadening so this cannot be ruled out, especially because there is a large temperature gradient in the coolant from BOC to EOC. Secondly, the amount of energy groups used by WIMS in its cross-section calculations may also impact how the criticality varies so little from BOC to EOC. This does not affect MCNP6 or SERPENT because of the continuous-energy libraries it uses.

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 optimization considering the fresh fuel isotopic composition and the geometry. It could ultimately be used as a supplementary tool in industry and regulation used in design, operation, trip coverage and safety margin analysis. It should be mentioned that preliminary results for the optimization algorithm will be demonstrated at the 12th Int. CANDU Fuel Conference Presentation.

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