FUEL COMPOSITION OPTIMIZATION IN A 78-ELEMENT FUEL BUNDLE FOR USE IN A PRESSURE TUBE TYPE SUPERCRITICAL WATER-COOLED REACTOR

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Abstract

A 78-element fuel bundlecontaining a plutonium-thorium fuel mixture has been proposed for a Generation IV pressure tube type supercritical water-cooled reactor. In this work, usinga lattice cell model createdwiththe code DRAGON,the lattice pitch, fuel composition (fraction of PuO_2 in ThO_2) and radial enrichment profile of the 78-element bundle is optimized using a merit function and a metaheuristic search algorithm.The merit function is designed such that the optimal fuel maximizes fuel utilization while minimizing peak element ratings and coolant void reactivity. A radial enrichment profile of 10 wt%, 11 wt% and 20 wt% PuO_2 (inner to outer ring) with a lattice pitch of 25.0 cm was found to provide the optimal merit score based on the aforementioned criteria.

1. Introduction

Atomic Energy of Canada Limited (AECL®), in collaboration with Natural Resources Canada (NRCan) and the Natural Sciences and Engineering Research Council (NSERC), has developed a pre-conceptual SCWR design that is an evolution of the CANada Deuterium Uranium (CANDU®) reactor, utilizing both pressure tubes and a heavy water moderator[1]. This Pressure Tube type Supercritical Water-cooled Reactor (PT-SCWR), unlike a typical CANDU, features batch refueling, light water coolant and vertical fuel channels,while maintaining a low temperature and pressure heavy water moderator.

Initial physics studies in fuel design for the PT-SCWR concept have focused on maximizing fuel utilization (in the form of burnup in Megawatt·days per tonne of initial heavy elements) while at the same time ensuring a negative coefficient of Coolant Void Reactivity (CVR)[2]. Additionally, the nuclear fuel itself is to contain the fertile isotope ^{232}Th, which breeds to the fissionable isotope ^{233}U. A 78-element fuel bundle design has thus been proposed, containing a reference fuel composition of 13 weight per cent PuO_2 in ThO_2, established concurrently with a lattice cell spacing of 25 cm [3]. Nevertheless, alternative designs utilizing different weight fractions of PuO_2 in ThO_2 in each ring of elements, as opposed to a single uniform composition across the entire bundle, can provide superior fuel performance with respect to discharge burnup, CVR and peak Linear Element Ratings (LERs)[4]. The objective of this study is therefore to optimize the fuel composition in each ring of elements in the 78-element bundle, concurrently with the lattice cell spacing, subject to the previously established design constraints.

2. Modelling and Optimization Methodology

A model of the 78-element fuel lattice cell was created using DRAGON 3.06J, a neutron transport code used for steady-state and slowly time-variant (e.g. isotopic depletion or burnup)

reactor lattice cell calculations [5]. Nuclear data was taken from the 69 energy group WIMSD library released by the International Atomic Energy Agency (IAEA) [6]. All geometry and material properties were consistent with previous studieswith the exception of the presence of yttrium in the ceramic insulator of the channel [3,7,8].Yttrium is not included in the IAEA libraries, and thus the balance of material within the ceramic insulator was modelled as zirconium.The spatial meshing for the DRAGON model is shown in Figure 1.

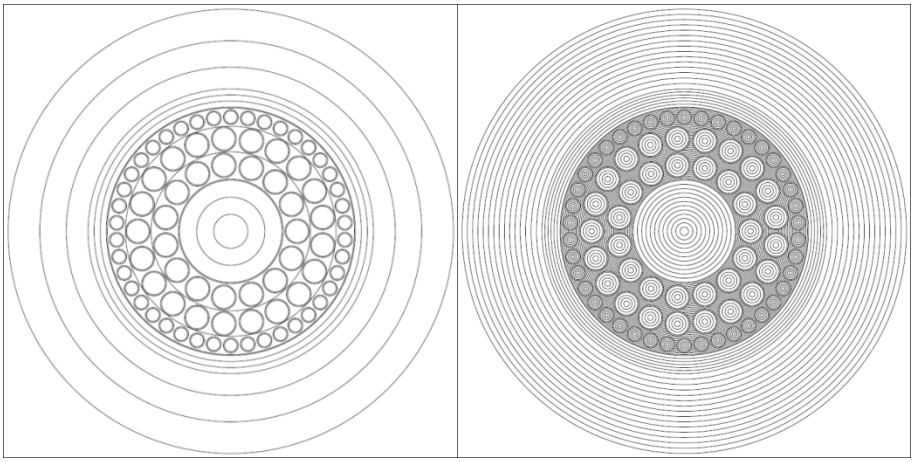

Figure 1 DRAGON lattice cell for self-shielding (left) and flux (right) calculation

Owing to the significant change in coolant properties expected along the length of a PT-SCWR channel, several two-dimensional lattice cell models are necessary to accurately capture the fuel behaviour as a function of axial position. As with previous studies, five equally spaced locations are modelled (0.5 m, 1.5 m, 2.5 m, 3.5 m and 4.5 m along the channel), where the average infinite neutron multiplication factor k_{inf}, discharge burnup and CVR among these five locations are sufficiently descriptive of the channel average [7,4,8].The relative ring powers determined from the DRAGON output are also normalized to the expected beginning-of-cycle axial power profile of the PT-SCWR to determine the peak initial LERsat the aforementioned positions [7].

The number of potential combinations of Pu/Th in each ring and lattice spacing can, depending on the size and resolution of the allowed search space, range from several hundred to hundreds of thousands of unique permutations, making the brute force simulation of every possible fuel design impractical with commonly available computational tools. Instead, a heuristic or computational metaheuristic algorithm is needed to drastically decrease the number of simulations needed, and therefore the computational time required while still providing high confidence that an optimal solution is obtained. The “Bees Algorithm” is a metaheuristic algorithm used for solving complex multivariable functional and combinatorial optimization problems based on the food foraging behaviours of honey bees, and is part of the larger class of well-known swarm-based optimization algorithms based on natural processes, including the Genetic Algorithm, Ant Colony Optimization and Particle Swarm Optimization [9]. The algorithm is as follows:

1. The search population is initialized with n random solutions produced by n independent workers (the eponymous “bees”).

2. The fitness of each solution is evaluated using an objective function, assigning each a value of merit.
3. While the stopping criteria are not met:
    a. The best m solutions from the population of n are selected for a "neighbourhood" search, and the best e "elite" solutions are selected from the population of m.
    b. nep solutions are found randomly in the neighbourhood of each "elite" site, and nsp solutions are found in the neighbourhood of each of the remaining $(m - e)$ selected sites.
    c. The remaining $(n - m)$ workers find solutions randomly over the entire search space.
    d. The fitness of all the new solutions is evaluated using the objective function.
    e. Determine if the stopping criteria are met, and if not return to a. for the next iteration.

To perform the optimization it is necessary that each simulated fuel composition be assigned a figure of merit. Similar to past fuel optimization studies, and in accordance with the goals of GIF, fuel performance is evaluated on the basis of discharge burnup, coolant void reactivity and maximum initial linear element rating. Each of these parameters serves as an input to an objective function(1), allowing the optimization algorithm to search for the fuel composition that provides the maximum merit value (i.e. the optimal composition). Each of the individual terms in (1) is itself a function between zero and one. Weighting factors are also implemented to adjust how quickly each term changes, however in this study each was left at its default value of w = 1.0.

$$\text{Merit} = 100 \times \left(\frac{e^{-\frac{(\text{Burnup}-4.5\times10^4)^2}{(2.0\times10^4)^2}}}{1+e^{(\text{Burnup}-6.0\times10^4)}} \right)^{w_1} \times \left(\frac{e^{\frac{\text{CVR}}{5}}}{1+e^{\frac{\text{CVR}}{0.001}}} \right)^{w_2} \times \left(\frac{1}{1+e^{\text{LER}-45}} \right)^{w_3} \qquad (1)$$

For this study the PuO_2 weight percentage in ThO_2 was treated as a separate variable in each ring of fuel elements, between values of 0 wt% and 20 wt%, in increments of 1 wt%. Furthermore, the lattice cell pitch (the distance between adjacent fuel channels) is also treated as a variable, between values of 22 cm and 27 cm, in increments of 1 cm. There are thus 55,566 unique permutations in this search space, requiring 277,830 DRAGON models. The brute force solution of every permutation in this search space would be computationally onerous, illustrating the need for a computational metaheurisitic algorithm.The "bees" algorithm was thus implemented via scripting on a Linux based computation server. The script, by generating the input files, calling DRAGON and parsing the outputs, returns the properties of the optimal fuel in each iteration of the algorithm (i.e. pitch, composition in each ring, burnup, CVR, LER and merit), ceasing execution once three iterations pass without an improvement in merit. Based on the available hardware, n = 64 workers were used, with the other parameters of the algorithm m = 6, e = 2, nep = 8 and nsp = 4.

3. Simulation Results and Analysis

It is noted from the description of the "bees" algorithm that there is a substantial amount of randomness in the progression of the optimization. It would be expected that, for three completely independent optimization runs on the same search space, the number of iterations required to reach the stopping criteria may be different and, given the metaheuristic nature of the algorithm, each may result in a different near-optimal solution. Three independent optimizations were thus executed for the defined fuel composition problem. Not only did each independent optimization run require a different number of iterations, but each resulted in a different optimal composition. The optimal composition from each run is thus presented separately in Table 1, along with the results of the reference fuel composition for comparison (note that the merit score for the reference fuel is zero owing to the positive calculated CVR).

Table 1Results of optimization algorithm

	Pitch (cm)	**PuO_2 Ring 1**	**PuO_2 Ring 2**	**PuO_2 Ring 3**	**Total PuO_2**	**Burnup ($MW \cdot d \cdot tonne^{-1}$)**	**CVR (mk)**	**Max.LER ($kW \cdot m^{-1}$)**	***Merit Score***
Run 1	25.0	10.0 %	11.0 %	20.0 %	13.14 %	44,499.32	-0.06	40.13	*98.02*
Run 2	25.0	15.0 %	9.0 %	18.0 %	13.26 %	42,035.24	-0.05	39.19	*96.51*
Run 3	25.0	7.0 %	13.0 %	19.0 %	12.80 %	43,159.62	-0.25	39.63	*93.85*
Reference	25.0	13.0 %	13.0 %	13.0 %	13.00 %	37,504.42	+0.14	35.41	*00.00*

Given that the values of burnup, CVR and maximum LER for the result of Run 1 reside very close to the peaks of the individual terms in (1), and on the merit scale of 0 to 100 it scores 98.02, it is reasonable to conclude that at the least Run 1 represents a very near-optimal result.

The three independent optimization runs cumulatively generated 1,569 unique DRAGON models, and thus much more simulation data than simply the optimal fuel is available. Fuel compositions with merit values greater than 50.00 can be taken as the subset of all near-optimal results, where generalizations about the qualities of near-optimal fuel compositions can be made. Of the 174 unique permutations modelled that fit this criterion, the following additional observations are made:

- 125 have a lattice pitch of 25.0 cm, and the remainder have a pitch of 24.0 cm. The truly optimal lattice spacing is therefore very likely to be near 25.0 cm.

- 123 contain 13.0 ± 1.0 wt% PuO_2 in the entire bundle. The optimal fuel loading for the entire bundle is therefore very likely to be near 13.0 wt%.

Taken together, these points would indicate that the optimal fuel would contain near 13.0 wt% PuO_2 over the entire bundle, and possess a lattice spacing of 24 to 25.0 cm. This is in fact very close to the definition of the reference fuel composition.The results of this optimization have shown, however, that how the 13.0 wt% is distributed among the three rings of elements can have a significant impact on the fuel performance.

4. Summary and Conclusions

Under the criteria of discharge burnup, coolant void reactivity and maximum initial linear element rating, the fuel composition and lattice spacing of a 78-element bundle fuelled with $PuO_2/ThO_2$for use in a PT-SCWR has been optimized. An optimal fuel composition of 10.0 wt%, 11.0 wt% and 20.0 wt% PuO_2 in the innermost to outermost rings of elements, respectively, with a lattice spacing of 25.0 cm was determined. This fuel loading provided a substantial improvement over the reference composition based on a predetermined function of merit. The reference composition of 13 wt% PuO_2 across the entire bundle and a lattice spacing of 25.0 cm were in fact maintained, with the improvement entirely attributable to the redistribution of PuO_2 among the rings of elements.

5. References

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