OPTIMIZATION OF THORIUM-URANIUM CONTENT IN A 54-ELEMENT FUEL BUNDLE FOR USE IN A CANDU-SCWR

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Abstract

A new 54-element fuel bundle design has been proposed for use in a pressure-tube supercritical water-cooled reactor, a pre-conceptual evolution of existing CANDU® reactors. Pursuant to the goals of the Generation IV International Forum regarding advancement in nuclear fuel cycles, optimization of the thorium and uranium content in each ring of fuel elements has been studied with the objectives of maximizing the achievable fuel utilization (burnup) and total thorium content within the bundle, while simultaneously minimizing the linear element ratings and coolant void reactivity. The bundle was modeled within a reactor lattice cell using WIMS-AECL, and the uranium and thorium content in each ring of fuel elements was optimized using a weighted merit function of the aforementioned criteria and a metaheuristic search algorithm.

1. Introduction

The next generation of nuclear fission reactors, as outlined by the Generation IV International Forum (GIF), is to feature enhanced safety, reliability, economics, sustainability and proliferation resistance relative to contemporary designs. In accordance with these goals and as a participant in GIF, Canada has chosen to focus its Generation IV research efforts on the Supercritical Water-cooled Reactor (SCWR) [1]. The SCWR, using high-temperature supercritical water as coolant, promises relatively high thermodynamic efficiency, and with a direct coolant cycle (thereby eliminating the need for steam generators) a significant economic advantage over current generation reactors [1].

Atomic Energy of Canada Limited (AECL®), in collaboration with Natural Resources Canada (NRCan) and the Natural Sciences and Engineering Research Council (NSERC), has developed several pre-conceptual SCWR designs that are evolutions of existing CANada Deuterium Uranium (CANDU®) reactors. As with existing CANDUs, these pre-conceptual CANDU-SCWRs are pressure tube type reactors with a heavy water moderator [2]. One particular pre-conceptual design features batch refuelling, light water coolant and vertical fuel channels, as opposed to online refuelling, heavy water coolant and horizontal channels in current generation CANDU. Additionally, this design includes a High Efficiency Channel (HEC), wherein a ceramic insulator within the pressure tube provides the necessary thermal isolation between the supercritical coolant and the low temperature moderator, eschewing the need for a separate calandria tube [2]. The current technical characteristics of this pre-conceptual design are summarized in Table 1.

Table 1: Technical characteristics of a pre-conceptual CANDU-SCWR [3]

Fuel Channels	336 vertical	**Coolant**	Supercritical H_20
Thermal Power	2,540 MW	**Pressure**	25 MPa
Moderator	D_2O	**Coolant Inlet**	367 °C; 0.55 g/cm^3
Refuelling	3-cycle batch	**Coolant Outlet**	597 °C; 0.08 g/cm^3

The evolution of the reactor thermalhydraulics has required equal advancement in the fields of fuel design and reactor physics. Several studies have been performed examining the effects of supercritical water coolant on existing CANDU fuel designs and entirely new fuel designs, consistent with the goals of the Generation IV program [3,4,5]. The objective of these studies has commonly been to examine:

- The inclusion of thorium to minimize the total uranium requirements, consistent with the goal for enhanced sustainability,
- Maximizing the fuel utilization (or "burnup", in the form of Megawatt-days per tonne of heavy elements), consistent with the goal for enhanced economics,
- Minimizing linear element ratings (in the form of kilowatts per metre), consistent with the goal for enhanced safety,
- Ensuring a negative coefficient of Coolant Void Reactivity (CVR), again consistent with the goal for enhanced safety.

Of particular interest, Boczar et al. detailed a 54-element fuel design (Figure 1), containing a large centre element intended to displace coolant, that could be used within a HEC in a CANDU-SCWR [4].

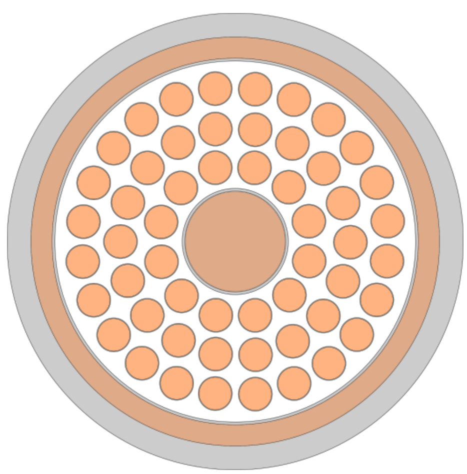

Figure 1: A 54-element bundle within a high efficiency channel

At the time, the extent of Boczar et al.'s study with the 54-element bundle was the relationship between potential burnup and CVR. Schofield meanwhile demonstrated that it was possible, at least in other (now obsolete) CANDU-SCWR fuel designs, to optimize different uranium and thorium enrichments in each ring of fuel elements for the purposes of maximizing burnup while simultaneously minimizing the surface heat flux and radial form factor [5]. The objective of this study was to therefore apply a similar methodology to the 54-element fuel design. In particular, the uranium enrichment and thorium content in each ring of fuel elements are examined on the basis of burnup, maximum linear element rating and CVR in order to find an optimal or near-optimal fuel composition for the 54-element bundle.

2. Methodology

2.1 WIMS-AECL Model Description

A model of the 54-element fuel within a HEC was created using WIMS-AECL version 3.1.2.2. WIMS-AECL is a two-dimensional neutron transport code used for steady-state and slowly time-variant (e.g. isotope depletion of "burnup") reactor lattice cell calculations [6]. Neutron cross-section data was taken from the ENDF/B-VII nuclear data library [7]. The dimensions of all elements, including the ceramic insulator and pressure tube, were consistent with those presented by Boczar et al. with the exception of the lattice cell spacing [4]. A lattice spacing of 22 cm was used rather than the 27 cm used by Boczar et al. in order to minimize CVR. This is within the range of potential lattice spacing values presented in previous studies [4,5].

The composition of all non-fuel materials within the lattice cell were also consistent with both the pre-conceptual design overview and previous fuel studies [2,3,4,5]. The pressure tube was composed of a zirconium based alloy called Excel. The cladding of the fuel elements and the liner tube covering the interior of the ceramic insulator were composed of 304L stainless steel. The ceramic insulator itself was composed of yttria-stabilized zirconia with 3 mol% Y_2O_3 and 20% porosity. By modelling the insulator as three separate annular regions, it was possible to represent the ingress of coolant through the porous material, linearly approximating the temperature of the mixture between the coolant and the moderator. The composition of the centre, coolant-displacing element has yet to be specified in literature, but given its intent it was assumed to contain solid zirconia for the purposes of this study. The fuel itself was modelled as a homogeneous mixture of thorium and uranium oxides, with the fraction of thorium to uranium in each ring of fuel elements and the uranium enrichment across the entire bundle (i.e. weight per cent of U^{235} relative to the total of U^{235} and U^{238}) used as variables in the optimization problem. This arrangement corresponds to a "once-through" thorium cycle, where the initial fissile content is entirely U^{235} which is eventually supplemented by the breeding of U^{233} from neutrons being absorbed in Th^{232}.

The heavy water moderator surrounding the pressure tube was assumed to be a uniform 80 °C. The properties of the supercritical light water coolant, however, vary considerably along the length of the channel (as shown in Figure 2). Therefore, for each unique fuel composition modelled, several WIMS-AECL models with different coolant properties were necessary to accurately characterize the fuel performance. Previous study has demonstrated that the average burnup of at least four evenly spaced simulation positions is well representative of the channel burnup as a whole, and this approach was used in this study as well [5].

Figure 3 shows the expected normalized axial power profile in a CANDU-SCWR channel for both the beginning (BOC) and end (EOC) of a batch refuelling cycle [3]. As shown in the figure, the beginning of the refuelling cycle will be the limiting case for thermal constraints (such as maximum linear element rating), and thus this was the power profile modelled using an expected maximum channel power of 9,648 kW [3].

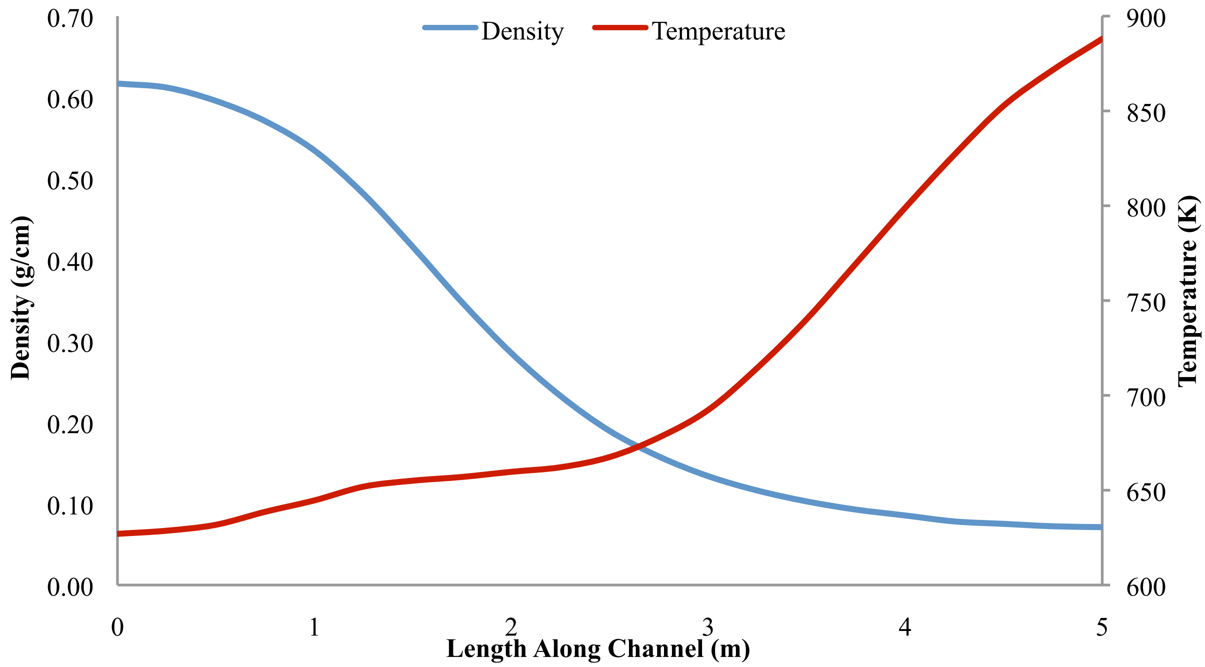

Figure 2: Supercritical water coolant properties [4]

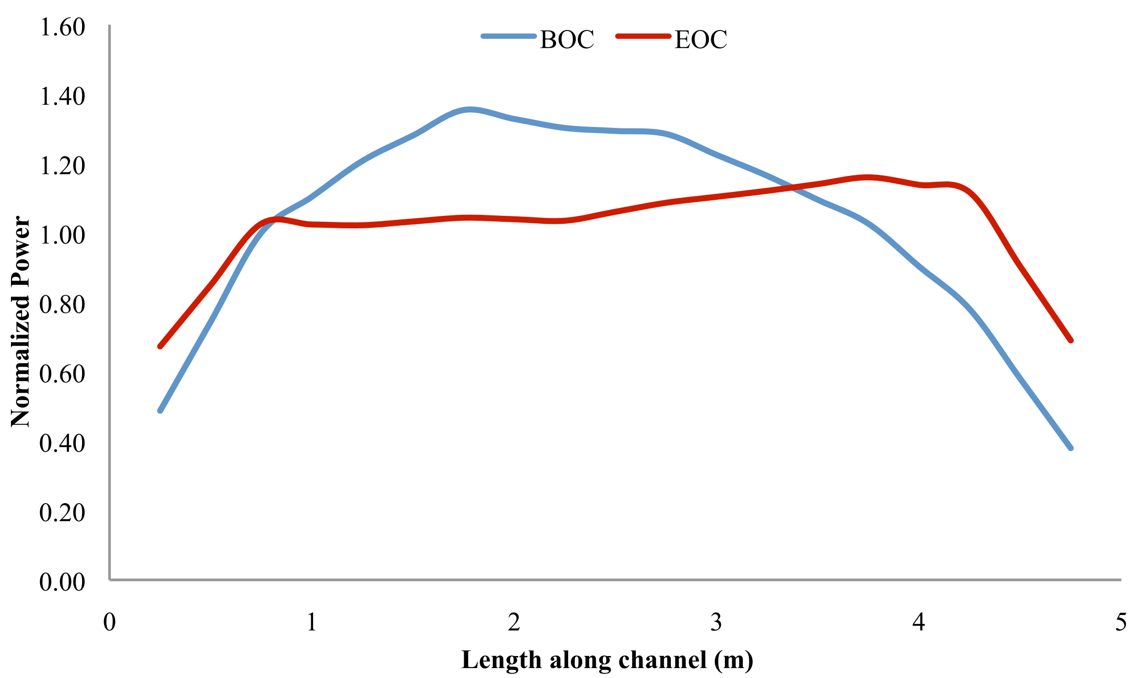

Figure 3: Normalized axial power profile [3]

In order to capture the power peak (and be consistent with the average burnups described above), the axial positions modelled in WIMS-AECL are located at 0.5 m, 1.5 m, 2.5 m, 3.5 m and 4.5 m along the length of the channel.

A convergence tolerance of 1.0×10^{-6} was used for the main transport solution. Burnup calculations were performed for five years of dwelling time within the reactor using time steps of ten days for most of the calculation (shorter time steps were chosen at the beginning). The maximum linear element rating was calculated at each time step, and the CVR every three time steps.

The value of burnup at discharge was taken at the point where the value of the instantaneous infinite neutron multiplication factor (k_{inf}) averaged over the aforementioned positions was exactly equal to 1.045. This value is an approximation of the excess reactivity in the core resulting from neutron leakage and absorption in materials not modeled in the lattice cell [4]. If this condition was not reached during the five year computation time, or if the fuel was never initially critical, that particular fuel composition was disregarded from further analysis. Although it is difficult to model a 3-batch refuelling scheme with a lattice code like WIMS-AECL, the linear reactivity model has previously been applied to estimate equivalent burnup values from lattice calculations [4]. By assuming a linear relationship between the fuel reactivity and burnup, this model allows quick determination of the relative change in discharge burnup for different numbers of batch refuelling cycles [8]. The lattice cell calculation used in this study is equivalent to single-batch refuelling, and application of the linear reactivity model indicates that the equivalent discharge burnup for a 3-batch refuelling scheme would be 150% of the single-batch cycle. The burnup values output by WIMS-AECL are thus adjusted by this amount.

2.2 The Bees Algorithm for Complex Optimization Problems

The number of potential combinations of thorium-uranium ratio and uranium enrichment in each ring of fuel elements (depending on the size and resolution of the search space, anywhere from several hundred to millions of unique permutations) make the brute force simulation of every potential fuel composition 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. The "Bees Algorithm" is a metaheuristic algorithm used for solving complex multivariable functional and combinatorial optimization problems (the latter being used in this study) based on the food foraging behaviour of honey bees, and is part of the larger class of swarm-based optimization algorithms based on observed 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* “bees”.
2. The fitness of each solution is evaluated using an objective function.
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 *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) sites.

c. The remaining (n - m) “bees” find solutions randomly in the entire search space.

d. The fitness of the new solutions is evaluated using the objective function.

2.3 Objective Function

Each fuel composition modelled is given a merit score (from 0 to 100) calculated from an objective (or "cost") function. In accordance with the design goals in previous reactor physics studies and the greater goals of the Generation IV program, the variables of the objective function include the thorium-uranium fraction within the entire bundle, the discharge burnup, the calculated coolant void reactivity (CVR) and the maximum linear element rating (LER), shown in (1). Each term in the objective function is also given a weighting factor $0 \leq w \leq 1$ to adjust its relative importance. The form of each term is shown graphically in Figure 4.

$$100 \times \left(\frac{Thorium\,Fraction}{100}\right)^{w_1} \times \left(\frac{Burnup}{40{,}000}\right)^{w_2} \times \left(\frac{e^{\frac{CVR}{5}}}{1+e^{\frac{CVR}{0.001}}}\right)^{w_3} \times \left(\frac{1}{1+e^{LER-45}}\right)^{w_4} \quad (1)$$

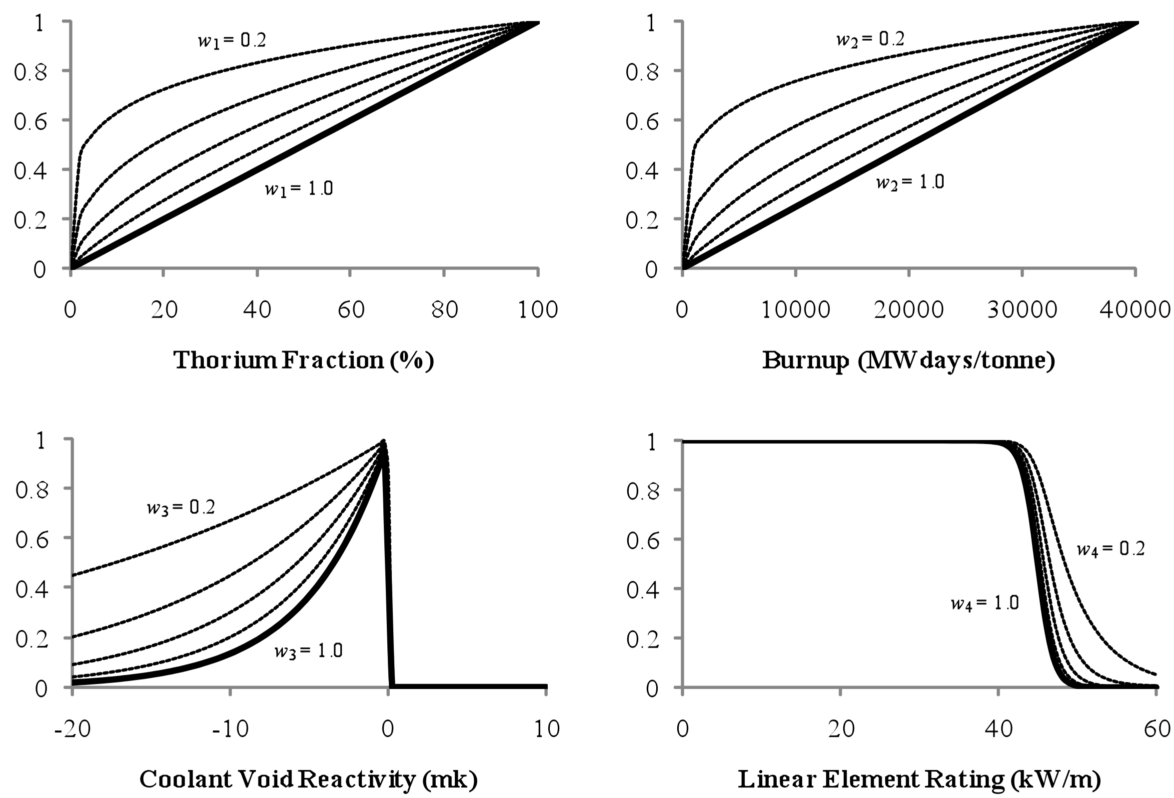

Figure 4: Individual terms in the objective function

The shape of each term was based on the various design goals presented in literature. Maximizing both the thorium utilization (requiring less uranium) and the discharge burnup have both been goals of physics studies, and in the case of the latter a target of 40,000 MW·days/tonne has been set [3]. A negative value of CVR has also been set as a design requirement, however at the same time it cannot be so negative that reactor stability and safety becomes a concern [4]. An acceptance criterion of 40 kW/m has also been set for the maximum linear element rating, beyond which the integrity of the stainless steel cladding becomes a concern at the target burnup [3]. However, in this study burnups less than the target are treated as acceptable (though not preferable), and so the constraint on LER is slightly relaxed.

2.4 Implementation of the Bees Algorithm for Fuel Optimization

The parameters for the bees algorithm were kept identical to the example presented by Pham et al. in their original paper [9]. There were n = 44 "bees" used in the computation. Of m = 3 best sites selected, e = 1 was chosen as an "elite" site. The size of each site or "patch" for the neighbourhood search was defined as within ± 2% U^{235} enrichment and ± 10% Th-U ratio. nep = 7 "bees" were sent to the elite site, and nsp = 2 "bees" were sent to each of the remaining (m-e) best sites. The remaining 33 "bees" were assigned to randomly search the solution space. The algorithm terminated when the best solution from the current iteration offered no relative improvement from the previous two iterations.

The algorithm was implemented in a script that was executed on a Linux-based computation server with 88 processors and 132 GB of physical memory. The script first generates and enumerates all possible permutations of fuel composition within the range of allowed values specified by the user. As a fuel composition is randomly selected by the algorithm for modelling, the script generates the necessary WIMS-AECL input files and submits them for execution to the computation server's job scheduler software. When the job scheduler gives the signal that the WIMS-AECL run is completed, the script opens the appropriate output file, extracting the required values and performing post-processing as needed for evaluation of the objective function. The script outputs the fuel composition with the best merit score from each iteration, as well as the value of each term in (1). The post-processed output of each fuel composition modelled is also kept in an output file, should they be required for future analysis.

3. Results

3.1 Algorithm Verification

A limited subset of potential uranium enrichments and thorium contents was initially chosen in order to verify the results of the optimization algorithm with a brute force computation (i.e. every permutation of fuel composition within the search space was simulated). For this verification study, the uranium enrichment was assumed to be constant over the entire bundle (one of 4%, 6%, 8% or 10% U^{235}), and each ring of fuel elements had one of six different thorium-uranium ratios (0%, 10%, 20%, 30%, 40% or 50% Th-U). There were thus 864 unique permutations, equivalent to 4,320 WIMS-AECL runs. In total, the brute force computation required 3.5 days of continuous computational time on the available computation server (approximately 75 minutes per each WIMS-AECL run). For this verification case, weighting values of w_1 = 0.4, w_2 = 0.8, w_3 = 0.2 and w_4 = 1.0 were chosen for the terms in the objective function.

With the results of the brute force computation, the first partial derivatives of the merit score with respect to each of the four design variables (uranium enrichment and the thorium fraction in each of the three rings of fuel elements) were determined. Multiple sign changes in the first derivatives indicated that there were several local maxima and minima in the solution space, indicating that a robust metaheuristic search algorithm such as the Bees Algorithm is needed for this type of optimization study. The global maximum (i.e. the optimal fuel design in this search space) occurred with a uranium enrichment of 10% U^{235}, 50% Th-U in the outermost ring of fuel elements and 0% Th-U in the two inner rings. The properties of this fuel as well as the respective contributions to the final merit score are shown in Table 2.

Table 2: Optimal fuel from brute force computation

Design Criteria	**Value**	**Term in (1)**
Bundle Thorium Fraction	22.0 %	0.5479
Discharge Burnup	45,961 MW·days/tonne	1.1175
Coolant Void Reactivity	-6.64 mk	0.7666
Max Linear Element Rating	50.41 kW/m	0.0044
Overall Merit Score from (1)		**0.2085**

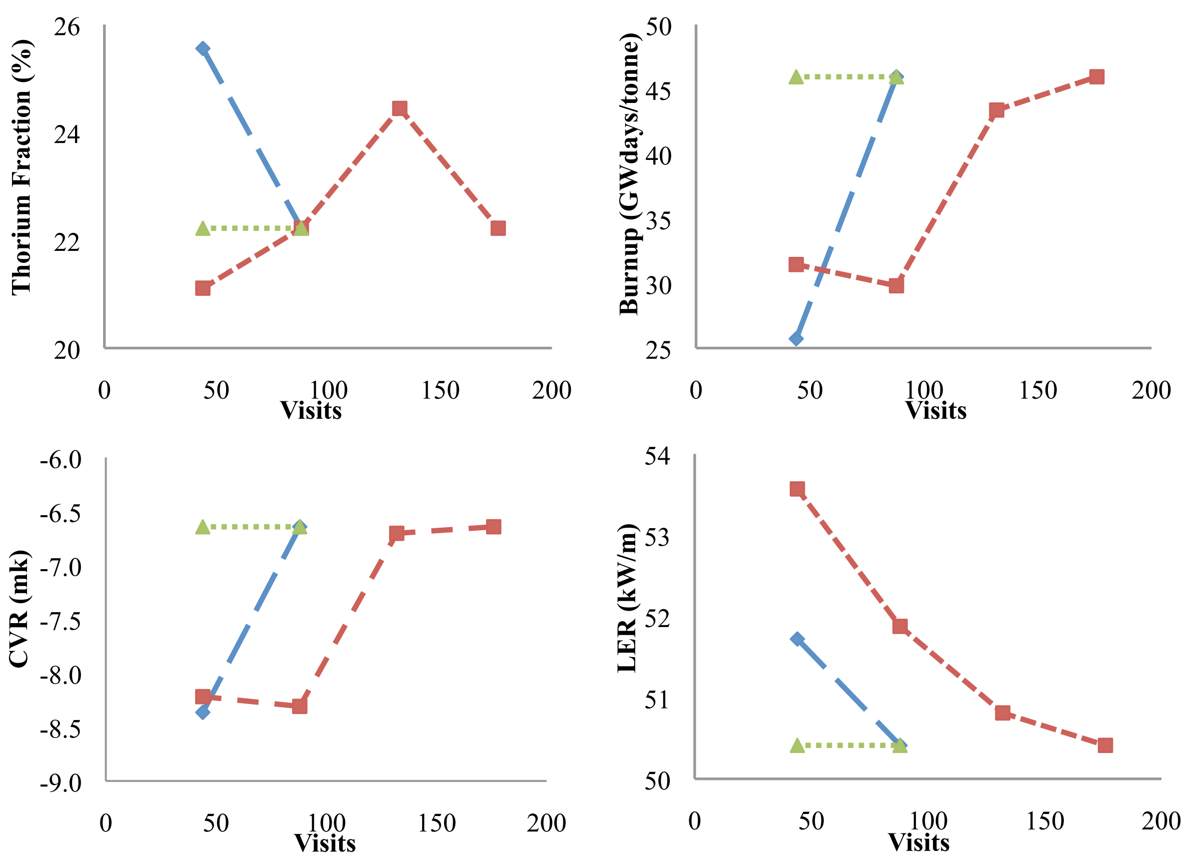

Figure 5: Evolution of the design criteria for three different runs of the Bees Algorithm

There is an element of randomness to the Bees Algorithm, and therefore it was expected that multiple independent searches of the same space may take a different number of iterations to converge to the same solution. Three different runs of the Bees Algorithm were thus executed over the space used in the verification study. The evolution of the optimal fuel is shown in Figure 5, where a "visit" by a worker bee denotes the simulation of a fuel composition.

In each case, the Bees Algorithm successfully delivered the optimal fuel composition described in Table 2 as determined by the brute force computation (i.e. 10% U^{235}, 50% Th-U in the outermost ring of fuel elements and 0% Th-U in the two inner rings). In one case the optimal fuel was found in four iterations of the Bees Algorithm (equivalent to 176 "visits" as defined by the number of "bees" *n* used in the computation), in another case two iterations (88 "visits") were required, and in the final case the optimal fuel was found with only one iteration (44 "visits", although the algorithm as written will always require at least two iterations to determine the optimal solution). In the slowest case, 176 "visits" only represents approximately 20% of the entire search space (864 unique permutations), and thus a significant improvement in computation time over the brute force computation.

3.2 Fuel Composition Optimization

For the full fuel optimization study, a much larger search space was used than in the verification case. Uranium enrichment was allowed to vary from 8% to 14% U^{235} in increments of 2%, and the thorium fraction in each ring of fuel elements was allowed to vary from 0% to 100% in increments of 10% Th-U. This space included 5,324 unique permutations of fuel composition, which would require 26,620 runs of WIMS-AECL to simulate entirely (thus precluding the brute force computation of the entire search space for verification purposes). The parameters in the Bees Algorithm and the weighting vales for the objective function were identical to those used in the verification study.

Execution of the Bees Algorithm returned a fuel composition in three iterations that was 14% U^{235} and contained 10%, 40% and 70% thorium in rings two, three and four respectively. The properties of this fuel and the contributors to the final merit score are shown in Table 3.

Table 3: Design values for "optimal" 54-element Uranium-Thorium fuel

Design Criteria	**Value**	**Term in (1)**
Bundle Thorium Fraction	46.7 %	0.7373
Discharge Burnup	36,675 MW·days/tonne	0.9329
Coolant Void Reactivity	-6.42 mk	0.7736
Max Linear Element Rating	47.78 kW/m	0.0584
Overall Merit Score from (1)		**3.1082**

3.3 Analysis of Fuel Performance

The most striking observation from both the verification study and the full optimization search is the dominance of the maximum linear element rating term. In each case, the algorithm could not find an acceptably low value for peak LER that does not drag down the objective function, resulting in very low values of merit (on a scale of 0 to 100) for even the "optimal" fuel design. This indicates there may be an issue with the peak LERs in the 54-element fuel bundle design that is not be resolvable by optimizing fuel composition alone. Evidently, the algorithm attempts to lower the peak LER by placing more thorium where the thermal neutron flux (and in homogeneous fresh fuel, the power generation) is highest, in the outermost ring of fuel elements. In this way, the thorium in the outermost ring in fresh fuel is acting as a localized burnable "poison" that later in life becomes fissile U^{233}.

In each case, the algorithm also selected the highest value of U^{235} enrichment allowable in the search space specified. This is to be expected in the once-through-thorium (OTT) cycle that was assumed in this study, and given the formulation of the design goals. Higher uranium enrichment provides more initial fissile inventory in the fuel, allowing both higher thorium-uranium ratios and discharge burnups to be achieved. Note that this is always true when the uranium enrichment varies uniformly over the entire bundle. If the uranium enrichment was also allowed to vary by ring, different enrichments in different rings may produce superior fuel performance (as was the case with the thorium fraction in the outer ring relating to the peak LERs). In further optimization study, it could thus be assumed that unless the uranium enrichment does vary by ring, that the highest allowable value will produce the optimal result.

4. Conclusions

The thorium content and uranium enrichment in a CANDU-SCWR 54-element fuel bundle has been studied for the purposes of optimizing fuel performance under the criteria of total thorium content, discharge burnup, coolant void reactivity and maximum linear element ratings. Given the large number of design variables and the size of the search space, a metaheuristic combinatorial search algorithm was needed. An algorithm based on the food foraging behaviour of honey bees (the "Bees Algorithm") was used to operate on a WIMS-AECL model of a CANDU-SCWR lattice cell to find the uranium enrichment and thorium content in each ring of fuel elements that provided the optimal merit score from a specified objective function.

For a limited search space, the results of the optimization algorithm were first verified against the brute force computation of all unique permutations of fuel composition to establish that the algorithm was capable of locating the optimal result. The optimization algorithm also provided a significant reduction in required computation time relative to the brute force solution. A much larger optimization study was then executed, resulting in an "optimal" fuel design that contained 14% U^{235}, with 10%, 40% and 70% thorium in rings two, three and four respectively.

In both the verification and optimization cases, it was found that the peak linear element ratings were dominating the objective function, resulting in relatively low values of merit for even the optimal fuel compositions. The 54-element fuel bundle design evidently provides peak element ratings in excess of the design objectives that are not resolvable by optimizing fuel composition in the rings of elements alone. For future work, a similar optimization study will be performed on the latest conceptual 78-element fuel bundle for CANDU-SCWR, which was designed to possess much lower peak LERs than the 54-element bundle concept [3].

5. References

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