Non-Parametric Study on the Optimization of Thorium 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 Supercritical Water-Cooled Reactor, a conceptual evolution of existing CANDU® reactors. Pursuant to the goals of the Generation IV International Forum, specifically regarding advancement in fuel cycles, the feasibility of optimizing the thorium content within each ring of fuel elements has been studied. 864 unique permutations of thorium and uranium content were modeled with WIMS-AECL, and the results were analyzed using non-parametric statistical methods. Key findings include that discharge burnup and coolant void reactivity are inversely related to the total thorium content in the bundle, and that the maximum linear rating and form factor are inversely related to the thorium content in the outermost ring of fuel elements.

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 modern designs. In accordance with these goals and as a participant of GIF, Canada has elected 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 CANDU reactors, these pre-conceptual CANDU-SCWR designs are pressure tube type 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 CANDUs. Additionally, this design includes a new High Efficiency Channel (HEC), wherein a ceramic insulator within the pressure tube provides the thermal isolation between the supercritical coolant and the low temperature and pressure moderator, eschewing the need for a separate calandria tube [2]. The technical characteristics of this pre-conceptual design are summarized in Table 1, and it serves as the basis for this study.

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

Fuel Channels	300 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 objectives of these studies have 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 including both uranium and thorium), consistent with the goal for enhanced economics,
- Minimizing the linear element rating and the variation in power generation rate (or "form factor") within the fuel bundle, 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 new 54-element fuel design (Figure 1), containing a large centre element intended to displace coolant, that could be used within a HEC in a pre-conceptual CANDU-SCWR [3].

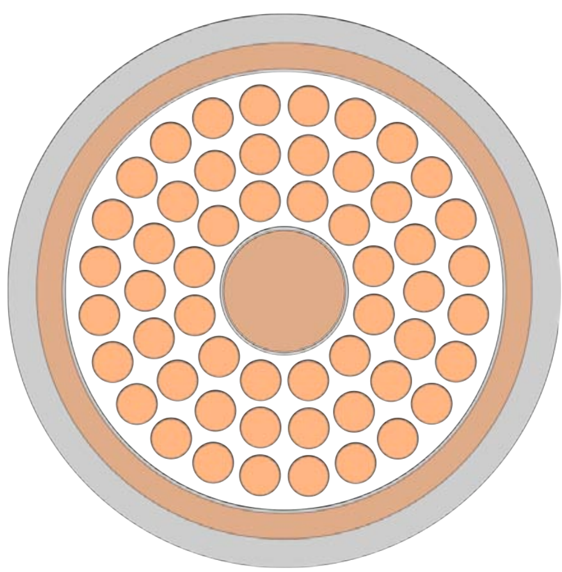

Figure 1: 54-element bundle contained within a HEC.

At the time, the extent of Boczar et al.'s study with the 54-element fuel 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 varying uranium and thorium enrichments in each ring of fuel elements within the fuel bundle for the purposes of maximizing burnup while simultaneously minimizing the surface heat flux and form factor [4]. The objective of this study is therefore to apply a similar methodology to the 54-element fuel design. In particular, several different combinations of uranium enrichment and thorium content within the rings are examined on the basis of burnup, linear element rating, form factor and CVR to determine the feasibility of this type of optimization for the 54-element fuel.

2. 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 or "burnup") reactor lattice cell calculations. Neutron cross-section data was taken from the ENDF/B-VII nuclear data library. 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 [3]. Given the different fuel compositions in the current work, the lattice spacing had to be reduced from the 27 cm used by Boczar et al. to ensure a negative value of CVR. A value of 22 cm was used instead, which is within the range of potential lattice spacing presented in previous studies [3,4,5].

The general 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]. The pressure tube was composed of a zirconium based alloy called Excel. The cladding of the fuel elements and the liner tube around 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_20_3 and 20% porosity. By modeling 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 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, where each increment along the abscissa is equivalent to the length of a typical CANDU fuel bundle). Therefore, for each unique fuel composition modeled, several WIMS-AECL models with different coolant properties were necessary to accurately characterize the fuel performance. It was previously demonstrated that the average burnup of positions two, five, eight and eleven is well representative of the channel burnup as a whole, and this approach was used in this study as well [4].

The fuel itself was modelled as a homogeneous mixture of uranium and thorium oxides. To focus specifically on the effects of varying the thorium content within the rings, and to limit the number of variables, the value of uranium enrichment for each case was uniform over the entire bundle (one of 4%, 6% 8% or 10% U^{235}). One of six different values of thorium-uranium ratio was chosen for each ring of fuel elements (0%, 10%, 20%, 30%, 40% or 50% Th^{232}). There were therefore 864 unique permutations modelled, and with four positions along the channel for each case, a total of 3,456 WIMS-AECL computations.

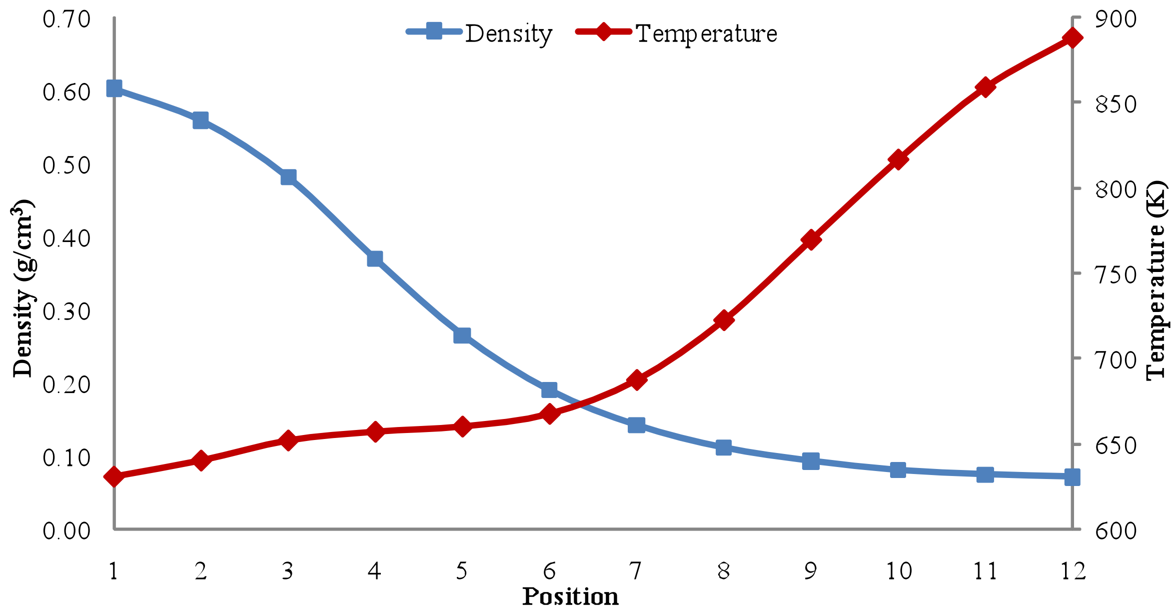

Figure 2: Supercritical water coolant properties [3].

Using 89 energy groups, 68 solution tracking lines at 19 angles were specified within the channel region, and an additional 42 lines at 19 angles in the moderator region. A convergence tolerance of 1.0×10^{-6} was used for the main transport solution. Assuming a channel length of 6 m and a flat power distribution along the length of the channel, the values of Table 1 were used to specify an average power of 14,111 W/cm. Burnup calculations were performed for five years of dwelling time within the reactor using time steps of ten days. The maximum linear element rating and form factor was calculated at each timestep, and the CVR every three time steps.

The value of burnup at discharge was taken at the point where the value of the infinite neutron multiplication factor (k_{inf}) averaged over positions two, five, eight and eleven 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 [3]. If this condition was not reached during the five year calculation time, or if the fuel was never initially critical, that particular data point 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 [3]. 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 [6]. The type of 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 therefore be 150% of the values presented in this study.

3. Results and Analysis

From an engineering and design optimization perspective, it is useful to have knowledge of how changes in a particular design variable affect a design criterion or constraint. Spearman's rank correlation coefficient (commonly denoted ρ, however ρ' will be used to differentiate from reactivity) is a quantity in non-parametric statistics that describes how well a monotonic (though not necessarily linear) function relates two variables, without assuming a priori any relationships between the variables [7]. Values of ρ' range from $-1 \leq \rho' \leq 1$, where the closer ρ' is to -1 or 1 the closer the function is to monotonically decreasing or increasing, respectively, and ρ' values near 0 indicate no relationship between variables. Values of ρ' have been calculated for the four design criteria outlined above (i.e. discharge burnup, maximum linear element rating, maximum form factor and maximum CVR) to show how well they relate to changes in the thorium content in each of the rings of fuel elements, as well as the total thorium content within the bundle. These are presented in Table 2, where the bolded entries indicate strong relationships between variables (for the purposes of this study, $|\rho'| > 0.8$). To isolate any effects of the U^{235} enrichment, separate values of ρ' for each value of enrichment are presented.

Table 2: ρ' values for each design criteria as functions of thorium content

U^{235} Enrichment	Th^{232} Fraction	Burnup	Max. Element Rating	Max. Form Factor	Max. CVR
4%	Ring 2	-0.1760	0.3677	0.5360	-0.4873
	Ring 3	-0.3174	0.7144	0.6301	-0.5522
	Ring 4	-0.6717	**-0.8119**	-0.7547	-0.2623
	Total	**-0.9249**	0.1916	0.2529	**-0.9660**
6%	Ring 2	-0.1772	0.2793	0.3580	-0.3793
	Ring 3	-0.3530	0.4956	0.3906	-0.5424
	Ring 4	**-0.8343**	**-0.8712**	**-0.9024**	-0.5829
	Total	**-0.9765**	-0.2930	-0.3509	**-0.9743**
8%	Ring 2	-0.1874	0.3429	0.4487	-0.5044
	Ring 3	-0.3331	0.6831	0.5797	-0.6724
	Ring 4	-0.6028	**-0.8770**	**-0.8994**	-0.0047
	Total	**-0.9495**	0.0826	0.0420	**-0.9170**
10%	Ring 2	-0.1804	0.3654	0.5714	-0.5820
	Ring 3	-0.4029	0.6629	0.4500	-0.5468
	Ring 4	-0.4512	**-0.8115**	**-0.8321**	-0.1935
	Total	**-0.9137**	0.4395	0.4429	**-0.9336**

Well resolved inverse relationships exist between the total thorium content and the achievable discharge burnup, as well as the total thorium content and the maximum CVR. The former is shown graphically in Figure 3. There appears to be a close to linear inverse relationship between total thorium content and burnup, however at a given thorium content variations of up to 5,000 MW·days per tonne are possible by changing the relative fraction in each ring of fuel elements. This relationship holds true at each enrichment of U^{235}.

According to the values of ρ' in Table 2, there is also a relationship between the thorium fraction in the fourth (outermost) ring of fuel elements and the discharge burnup. This may be partially attributable to the fact that the fourth ring represents a greater fraction of the total mass of the bundle than the others, but more importantly the outer ring also sees the greatest thermal neutron flux, and thus possesses greater burnup than the others. This relationship is nonetheless shown graphically in Figure 4. It is evident that the variation in discharge burnup at a given total thorium content is mostly attributable to the relative fraction in ring four. Specifically, there is an inverse relationship between the thorium content in the outermost ring and burnup. The reason this relationship is less resolved at the lowest and highest U^{235} enrichment levels is likely due to lack of data, owing to the rejection criteria explained in the previous section. High levels of thorium with low U^{235} enrichment are likely to result in a fuel that is never initially critical. Similarly, low thorium content with a high U^{235} enrichment may result in fuel that does not reach the discharge condition ($k_{inf} \leq 1.045$) within the five year calculation time.

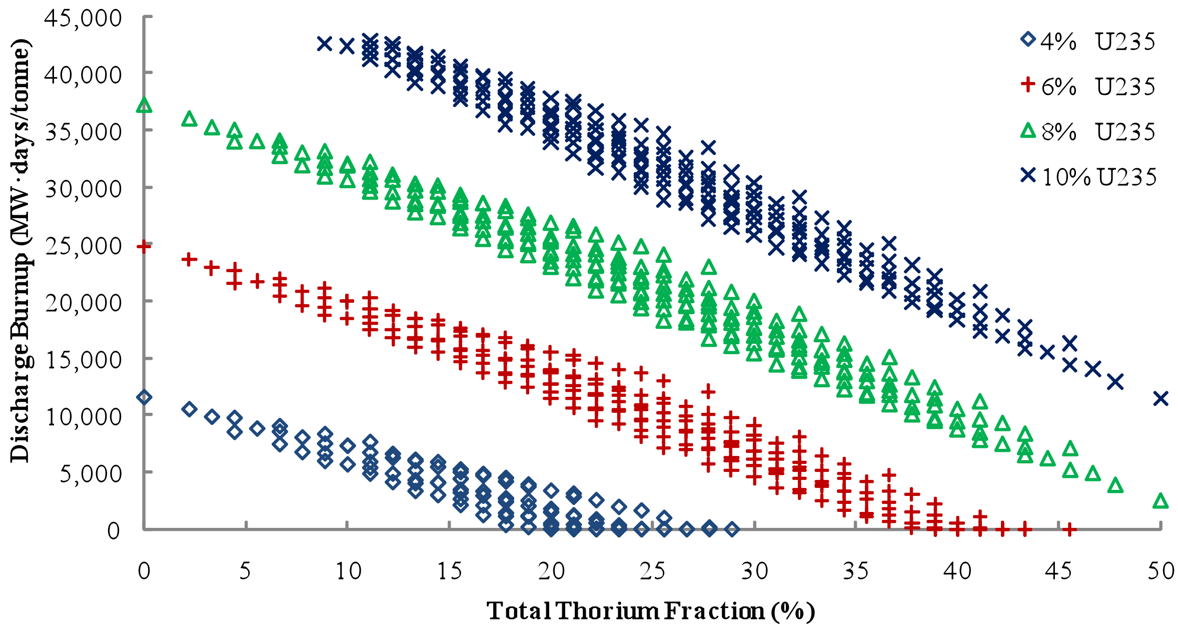

Figure 3: Achievable discharge burnup as a function of thorium content and uranium enrichment

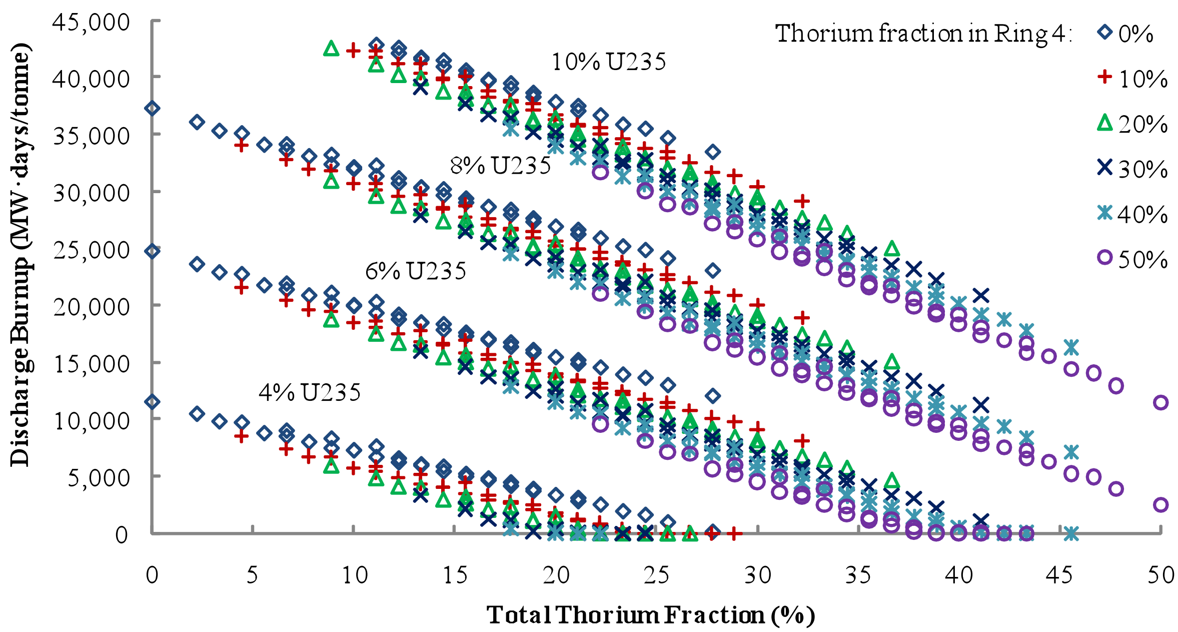

Figure 4: Discharge burnup as a function of total thorium content and content in ring four

The relationship between total thorium content and CVR is shown graphically in Figure 5. Again, there is a close to linear inverse relationship between total thorium fraction and CVR at each value of U^{235} enrichment. At a given value of total thorium content it also appears possible to vary the CVR by up to a milli-k by changing the relative fraction in each of the rings, however as indicated in Table 2 there are no well resolved relationships between the thorium content in any single ring and the CVR.

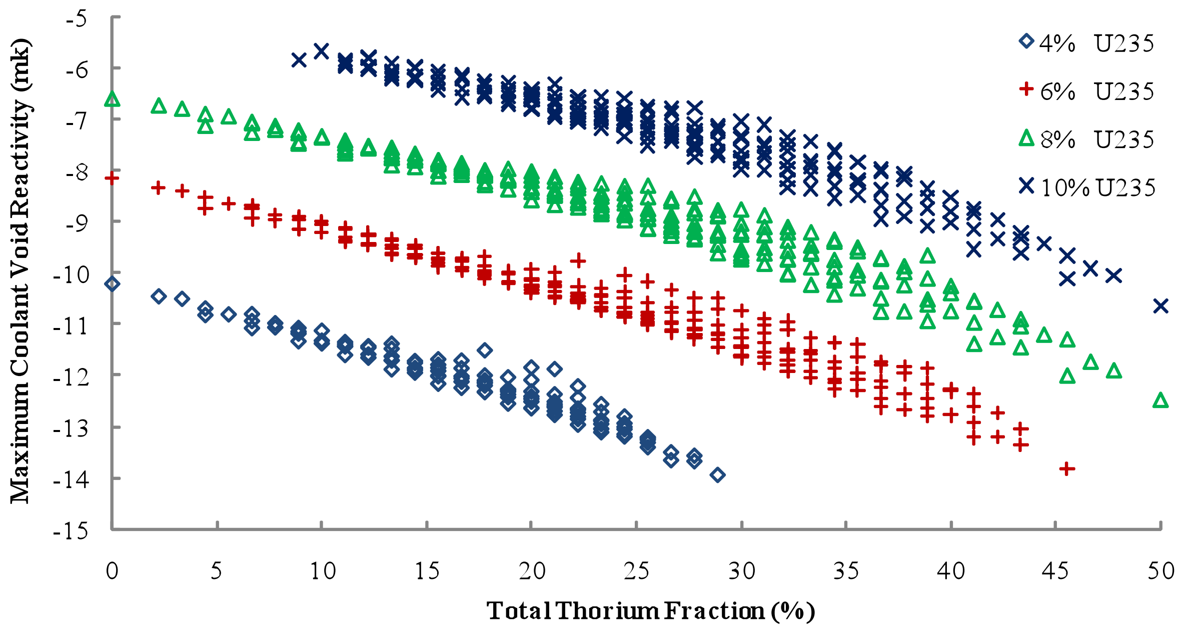

Figure 5: Maximum CVR as a function of thorium content

The maximum calculated linear element ratings and form factors are shown in Figures 6 and 7, respectively. It should be noted that since an average channel power and flat power distribution were used, the absolute value of the maximum linear element rating is expected to be smaller than more conservative estimates. However, any relationships gleaned from this non-parametric analysis are expected to hold true at any value of bundle power. As indicated by the values of ρ' in Table 2, the thorium content in rings two and three do not individually have a significant impact on the maximum linear element rating or form factor. There are, however, well resolved relationships between the maximum linear rating and form factor and the thorium content in ring four. The different values of thorium fraction are thus indicated on the following figures.

In Figure 6, each unique value of thorium content in ring four appears as a nearly distinct region. There are thus two observable relationships. First, an increased thorium content in ring four results in lower linear rating (consistent with the calculated values of ρ'). Second, when the thorium content in ring four is held constant but increased in the other rings, the maximum linear rating increases. This behaviour is consistent over the range of U^{235} enrichments used in this study. Given the increased neutron absorption that must occur in the inner rings when their thorium content is higher, and knowing that each WIMS-AECL model was normalized to the same power, this indicates that the maximum linear rating consistently occurs in the outer ring of fuel elements.

Figure 7 shows similar behaviour for the form factor. Again, consistent with the calculated values of ρ', there is an observable inverse relationship between the thorium content in ring four and the maximum form factor. Similar regions of unique thorium fraction exist, however there is much more overlap between these regions. This indicates that the form factor is in general less sensitive to the thorium content in ring four than the maximum linear rating. Nonetheless, the same logic can be used to deduce that the maximum power must occur in the outermost ring of fuel elements, consistent with the findings above.

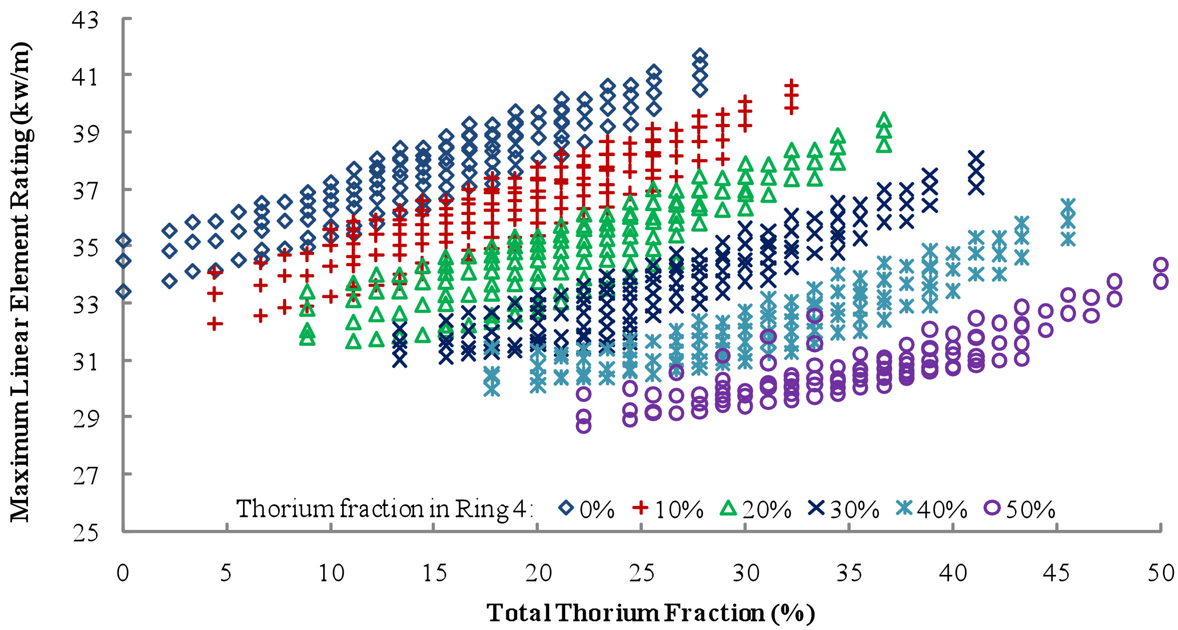

Figure 6: Maximum linear element rating as a function of thorium content

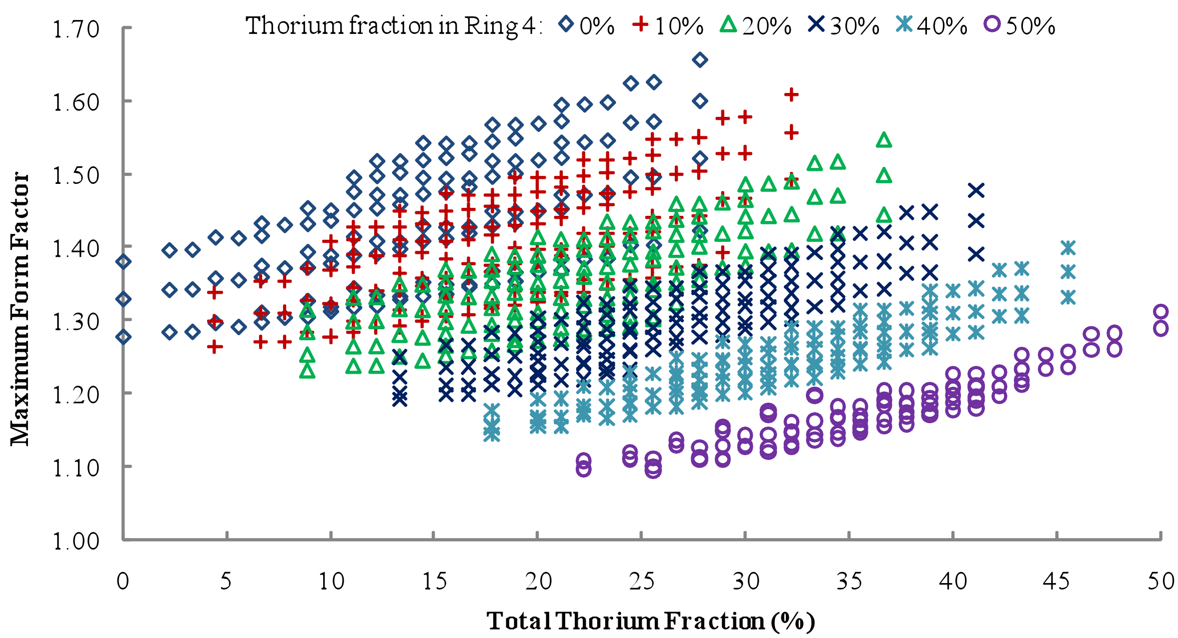

Figure 7: Maximum form factor as a function of thorium content

4. Conclusions

The feasibility of optimizing the thorium content in the rings of a 54-element bundle in a CANDU-SCWR has been studied using non-parametric statistics under the criteria of discharge burnup, coolant void reactivity, linear element rating and form factor. Several relationships have been gleaned from this analysis that indicate that this sort of optimization is possible. First, it was found that increasing the total thorium content in the fuel, and to a lesser extent in the outermost ring of fuel elements, decreases the realizable discharge burnup. This is an undesirable result for the purposes of economics. Conversely, increasing the total thorium content decreases the coolant void reactivity, which is desirable for safety. Further to the point of safety, it was found that increasing the thorium content in the outermost ring of fuel elements decreases the maximum linear element rating as well as the maximum form factor.

For a true design optimization it is still necessary to determine decision weighting factors for each of the aforementioned criteria, which is beyond the scope of this study. However, with the above relationships established, it is now possible to create a heuristic optimization algorithm that does not rely on the brute force computation of every possible permutation of thorium and uranium compositions, but rather finds a optimal (or near optimal) design with much less computational effort. The results of this study indicate that an optimal fuel design would have greater thorium content in the outermost ring of fuel elements than in the interior rings, while simultaneously balancing the need for increased fuel utilization.

5. References

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