Lattice physics evaluation of 35-element mixed oxide thorium-based fuels for use in pressure tube heavy water reactors

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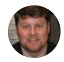

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LATTICE PHYSICS EVALUATION OF MIXED OXIDE THORIUM BASED FUELS FOR USE IN PRESSURE TUBE HEAVY WATER REACTORS

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ABSTRACT

A series of 2-D lattice physics depletion studies were carried out as part of conceptual scoping studies to evaluate thorium-based fuels in Heavy Water Reactors. Fuel bundles used for the study consisted of 35 fuel elements arranged in two outer rings comprised of thorium mixed with a fissile driver of either reactor grade plutonium (3.5-4.5 wt% PuO_2), low enriched uranium (5 wt% $^{235}U/U$, 40-50 wt% $LEUO_2$) or uranium-233 (1.8 wt% $^{233}UO_2$). Lattice physics-based estimated for fuel temperature coefficients and coolant void reactivity values were found to be lower than those for conventional natural uranium HWR fuel. The low burnup LEU/thorium fuel bundle shows the most promise as a feasible means of generating U-233 in a PT-HWR from a safety and fuel performance perspective.

KEYWORDS: heavy water, thorium, lattice physics

I. INTRODUCTION

As a fertile nuclear fuel that is nearly three times as abundant as uranium, thorium shows great promise for long-term nuclear energy sustainability. Numerous papers have been written on the prospect of moving to a thorium-based fuel cycle, envisioning what could be accomplished in the future. In particular, the potential use of thorium-based fuels in pressure tube heavy water reactors (PT-HWR) has been a topic of in-depth study [1, 2, 3]. This paper outlines possibilities for gaining operational experience with thorium through the use of thorium based mixed oxide fuels in PT-HWRs. These reactors are attractive for implementation of advanced fuel cycles as they are an existing technology with high neutron economy, on-line refueling capability, and fuel flexibility.

Two-dimensional lattice physics calculations were performed for a number of thorium-based fuel bundle concepts, from which the various performance and safety characteristics were estimated. The key performance metrics (to be defined in section III) that were estimated include the conversion ratio (CR), the fissile inventory ratio (FIR), the discharge burnup (BU), the individual fissile isotope content, and the fissile utilization (FU). The key safety parameters that were estimated include the coolant void reactivity (CVR), fuel temperature coefficient (FTC), and the maximum linear element rating (LER).

II. PRESSURE TUBE HEAVY WATER REACTORS AND LATTICE CONCEPTS

Pressure Tube Heavy Water Reactors (PT-HWRs) differ from pressurized light water reactors in that they use pressure tubes in lieu of one large pressure vessel. Details about PT-HWR and their operational characteristics can be found in other works [4, 5]. In this study, the structural components of the fuel channel are similar to currently operating PT-HWRs [5]. Modelling parameters including temperatures, dimensions and materials for the various lattice components can be found in Table I and Table II.

Table I
Nominal Lattice Dimensions [6]

Dimension	Value (cm)
Lattice pitch	28.575
Pressure Tube Inner Radius	5.1689
Pressure Tube Outer Radius	5.6032
Calandria Tube Inner Radius	6.4478
Calandria Tube Outer Radius	6.5875

Table II
Nominal Material Specifications [6]

Structure	Temp. (K)	Material	Density (g/cm^3)
Coolant	561	99.1 wt% D_2O	0.808
Pressure Tube	561	Zr-2.5Nb	6.515
Gap	451	CO_2	0.0012
Calandria Tube	342	Zircaloy-2	6.544
Moderator	342	99.7 wt% D_2O	1.085

The bundle geometries modeled in this case shall be referred to as BUNDLE-37 and BUNDLE-35. The BUNDLE-37 geometry is similar to a conventional 37-element natural uranium

PT-HWR fuel bundle. Zircaloy-4 is used as the fuel sheath material and the sheath surrounds the sintered fuel pellets. BUNDLE-37 has 37 fuel elements arranged in four rings, as seen in Figure 1.

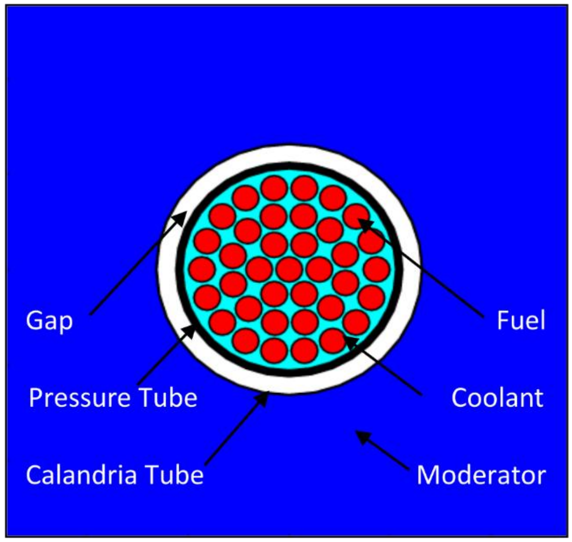

Figure 1: BUNDLE-37 Geometry

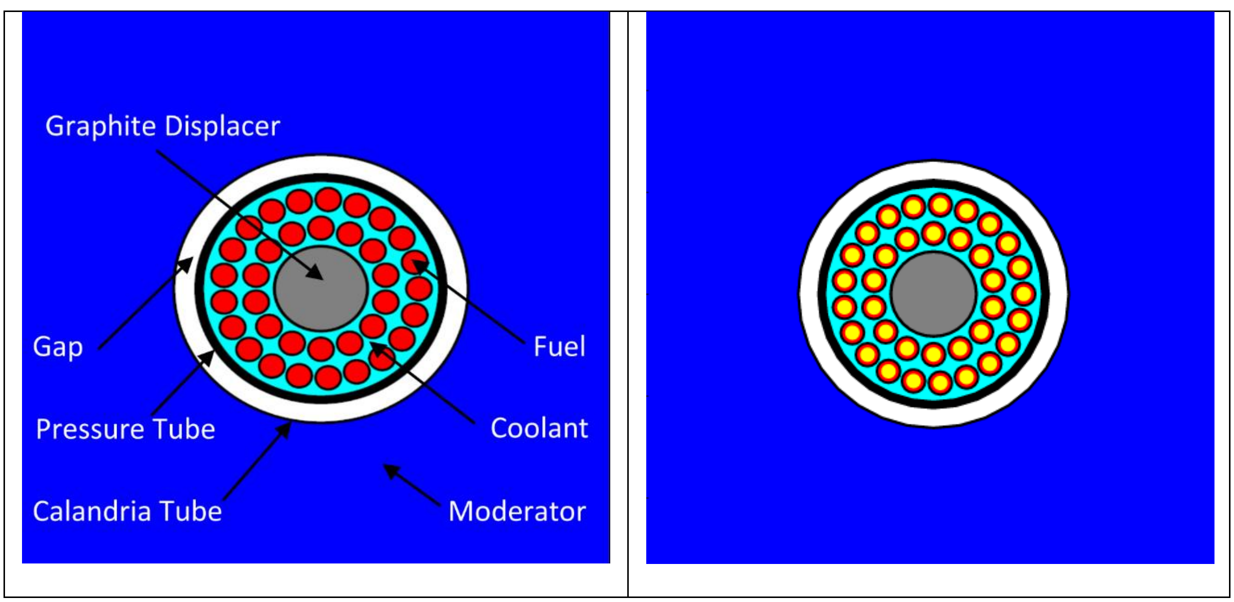

Figure 2: BUNDLE-35 Uniform Fuel Geometry (left) and Duplex Geometry (right)

The other fuel assembly studied is the BUNDLE-35 concept, consisting of two rings of fuel elements surrounding a central graphite displacer rod as shown in Figure 2. There are two types of fuel pellet geometry studied in this fuel bundle type, with a homogeneous fuel (left) Figure 2, and a duplex fuel (right) Figure 2. The Duplex fuel elements consist of a core of pure thorium and the fissile fuel component mixed with thorium in the outer fuel annuli. The BUNDLE-35 concept also includes small amounts of thorium dioxide in the last 3 cm of fuel pellets to axially grade the fissile content of the fuel bundle to reduce axial power peaking. The amount of thorium used in the last 3 cm of end pellets on either side of the fuel stack is approximately equivalent to 2 vol% in the entire fuel stack, modelling this in 2D requires some approximations discussed later in the text. The geometry specifications for the fuel can be found in Table III. The material specifications, densities, and bundle powers used for burnup calculations and linear element rating estimates can be found in Table IV. A nominal fuel bundle power of 600 kW is used for 2-D lattice cell burnup calculations and 3-D fuel bundle simulations. This corresponds approximately to the flux-squared-mean bundle power that would be found in the core of a conventional 700-MW_e-class PT-HWR operating at 2,061 MW_{th}, with 380 fuel channels and 12 bundles per channel [5]. The peak bundle power in a typical PT-HWR will range from 800 kW to 900 kW [7, 8]. The fuel, sheath, and coolant temperatures chosen are approximate values, and are treated as uniform throughout the bundle. The temperature of the ThO_2 in the central fuel element has been set to match the uranium-based fuel throughout the rest of the bundle, although it is expected to be lower due to the lower power level in the thorium fuel element and the higher thermal conductivity of ThO_2. This will under predict the amount of ^{233}U produced in the central element because a higher temperature effectively suppresses reactivity due to fuel temperature feedback, additionally the exit burnup of the fuel overall may be conservative for the same reason.

Table III
BUNDLE-35 Geometry Specifications

Quantity		Value	Units
Dimensions			
Length of Fuel Bundle		49.53	cm
Length of Fuel Stack		48.0	cm
Number of Fuel Elements		35	ele
Duplex Fuel Pellet Inner Radius		0.375	cm
Fuel Pellet Outer Radius		0.530	cm
Fuel Element Outer Radius		0.574	cm
Ring 1	Fuel Elements	14	ele/ring
	Pitch Circle Radius	2.97	cm
	Angular Offset	12.59	degrees
Ring 2	Fuel Elements	21	ele/ring
	Pitch Circle Radius	4.38	cm
	Angular Offset	0	degrees

Table IV
BUNDLE-35 Fuel Bundle Material Specifications

Quantity	Value	Units
Temperatures		
Fuel	941	K
Central Graphite Displacer	561	K
Materials		
Sheath	Zircaloy-4	
Displacer	Graphite	
Densities		
Zircaloy-4 in Fuel Sheath	6.464	g/cm^3
Graphite in Central Displacer	1.5	g/cm^3
Uranium-based Fuel	10.00	g/cm^3
Thorium-based Fuel	9.70	g/cm^3
Bundle Masses		
Nominal Bundle Heavy Element Mass	13.055	kg
Bundle Powers		
Average Power	600	kW
Specific Power in Fuel	45.96	kW/kgHE

Table V
Fuel Material Specifications

Fuel Type	Nuclide	Nuclide Amounts (wt%)	Theoretical Density (g/cm^3)	Effective Modelled Density (g/cm^3)
Natural UO_2	U234	4.68E-03	10.97	10.0
	U235	6.27E-01		
	U238	8.75E+01		
	O16	1.18E+01		
	O17	4.79E-03		
LEU (5 wt% $^{235}U/U$)	U234	3.37E-02	10.97	10.0
	U235	4.42E+00		
	U238	8.40E+01		
	O16	1.19E+01		
	O17	4.81E-03		
ThO_2	TH232	8.79E+01	10.0	9.7
	O16	1.21E+01		
	O17	4.89E-03		
PuO_2	PU238	2.43E+00	11.5	9.7
	PU239	4.58E+01		
	PU240	2.03E+01		
	PU241	1.34E+01		
	PU242	6.26E+00		
	O16	1.18E+01		
	O17	4.75E-03		
$^{233}UO_2$	U233	8.87E+01	10.97	9.7
	O16	1.13E+01		
	O17	4.92E-03		

The specifications of the various fuel bundle lattice concepts are given in Table VI, including the fuel composition, the bundle geometry, the pellet type (duplex or homogeneous), the relative power in the bundle, and the distributed thorium volume percent in the fuel. In a practical BUNDLE-35 fuel stack, up to 4% (by volume) of pure ThO_2 would be spread over the end region of the fuel (the last 3 cm of fuel pellets), and mixed homogeneously with the main mixed oxide fuel to effectively grade the fissile content and reduce power peaking in the end region. The effect of varying the distribution of thorium in the end pellets on end power peaking has been studied preliminarily for fresh uranium based fuels and the results are described in prior work [9].

The first lattice concept studied (LC-01) is the base case for comparison with the other lattice concepts. It consists of a 37-element geometry, filled with natural uranium dioxide fuel and is similar to a standard fuel bundle used in operating 700 MW_e PT-HWRs.

Lattice concepts LC-06b to LC-09b use $(Pu,Th)O_2$ fuel in a 35-element geometry. The fuel composition includes small amounts of reactor-grade plutonium (3.5 wt% and 4.5 wt%) as a fissile driver with the remainder consisting of thorium. Two of the concepts use homogeneous fuel pellets (LC-06b and LC-08b) and two use equivalent Duplex fuel pellets (LC-07b and LC-09b).

Lattice concepts LC-10b to LC-13b use $(LEU,Th)O_2$ fuel where the LEU is enriched with 5 wt% ^{235}U, also in the BUNDLE-35 geometry. The fuel compositions included 40 wt% and 50 wt% LEU as fissile driver, with the remaining oxides comprised of thorium. As with the previous concepts, two of the cases use homogeneous fuel (LC-10b and LC-12b), and two use Duplex elements (LC-11b and LC-13b).

Two (^{233}U,Th) lattice concepts (LC-14b and LC-15b) were studied in the BUNDLE-35 geometry with 1.8 wt% of $^{233}UO_2$ as the fissile driver. Concept LC-14b uses homogeneous fuel pellets and LC-15b uses Duplex fuel pellets.

Table VI
Lattice Concept Description

Lattice* Concept	Relative Power (W/gHE)	Bundle Geometry	Materials of Outer Fuel Rings	Duplex Fuel	Vol% ThO_2 End Pellets
LC-01	31.5	37-element	100 wt% NUO_2	No	—
LC-06b	45.96	35-element	3.5 wt% PuO_2 + 96.5 wt% ThO_2	No	4
LC-07b	45.96	35-element	3.5 wt% PuO_2 + 96.5 wt% ThO_2	Yes	4
LC-08b	45.96	35-element	4.5 wt% PuO_2 + 95.5 wt% ThO2	No	4
LC-09b	45.96	35-element	4.5 wt% PuO_2 + 96.5 wt% ThO_2	Yes	4
LC-10b	45.96	35-element	40 wt% $LEUO_2$ + 60 wt% ThO_2	No	4
LC-11b	45.96	35-element	40 wt% $LEUO_2$ + 60 wt% ThO_2	Yes	4
LC-12b	45.96	35-element	50 wt% $LEUO_2$ +50 wt% ThO_2	No	4
LC-13b	45.96	35-element	50 wt% $LEUO_2$ + 50 wt% ThO_2	Yes	4
LC-14b	45.96	35-element	1.8 wt% $^{233}UO_2$ + 98.2 wt% ThO_2	No	4
LC-15b	45.96	35-element	1.8 wt% $^{233}UO_2$ + 98.2 wt% ThO_2	Yes	4

III. EVALUATION CRITERIA

The lattice physics analyses performed will provide estimates of the reactor physics behavior at the full-core level. The specific evaluation criteria of the results are broken down into two categories: safety and performance.

III.A Operations and Safety Characteristics

The safety metrics evaluated for this study are: the infinite-lattice coolant void reactivity (CVR), the infinite-lattice fuel temperature coefficient of reactivity (FTC), and the maximum estimated linear element rating (LER). A discussion of how these parameters are calculated is given in prior work [9].

III.B Performance Metrics

The performance metrics evaluated here are the conversion ratio (CR), the fissile inventory ratio (FIR), the discharge burnup (DBU), the fissile nuclide content, the ^{233}U yield, and the fissile utilization (FU).

In this study, the discharge burnup is defined as the burnup at which the integrated k-infinity (or burnup-averaged k-infinity) is equal to 1.05 (evaluated in equation 5). It is assumed that an excess reactivity of approximately 50 mk (1 mk = 100 pcm = 0.001 $\Delta k/k$) will be lost due to neutron leakage and neutron absorption in reactivity devices (such as adjuster rods and liquid zone controllers) in the PT-HWR core [4]. The use of burnup-averaged k-infinity to determine the exit burnup is a good approximation for a nearly-continuously fuelled reactor.

$$\langle k_{\inf} \rangle = \frac{\int_{x=0}^{x=BU} k_{\inf}(x) \times dx}{BU} \tag{5}$$

The fissile inventory ratio (FIR) is the amount of fissile material in the fuel at an instantaneous burnup value divided by the initial amount. It is a measure of how much of the original fissile material has been spent and how much fissile material has been bred. Simply achieving a low FIR to ensure the initial fissile material is efficiently burned is not the target, since there is additional advantage to be gained by taking advantage of the fissile breeding potential associated with thorium-based fuel. To fully quantify the extent of breeding, the concentration of ^{233}U and other fissile nuclides are also examined in addition to calculating the FIR. Ideally, if there is significant breeding of new fissile material with a high conversion ratio, the fuel will achieve a high burnup, and it will also maintain a high FIR.

The fissile utilization is calculated as the discharge burnup divided by the initial amount of fissile material present in the fuel. The value examined in this case, however, is the relative fissile utilization, where for each concept it is normalized against the fissile utilization of natural uranium fuel in a PT-HWR (7.5 MWd/kg / 0.0071 weight fraction ^{235}U/U ≈ 1,056 MWd/kg-fiss) [10]. It is preferred to have a relative fissile utilization value greater than 1.0, indicating that a given fuel is performing as well or better than a large-scale natural uranium fuelled PT-HWR. Lastly, the conversion ratio is calculated by evaluating how much fissile material is produced at a particular point in time (through neutron capture by fertile isotopes, such as ^{232}Th, ^{234}U, ^{238}U, ^{238}Pu, and ^{240}Pu) divided by how much fissile material is depleted by fission, neutron capture or other reactions (such as n,2n).

III.C IV. COMPUTATIONAL METHODS AND APPROXIMATIONS

IV.A WIMS-AECL 2D Lattice Models

The lattice physics calculations were performed using WIMS-AECL Version 3.1 [11], a 2-D deterministic neutron transport code. An 89-group nuclear data library based on the ENDF/B-VII.0 [12] evaluation was used in conjunction with WIMS-AECL for this work.

As mentioned previously, details of the models that were prepared are given in Tables I to IV. The first case studied (LC-01) is considered the base case for comparison with the other lattice concepts. More information about the modelling methods and 3D approximations used in this work can be found in prior work [9].

Thorium dioxide has a theoretical mass density of 10.00 g/cm^3, plutonium dioxide has a theoretical mass density of 11.5 g/cm3, and uranium dioxide has a theoretical density of 10.97 g/cm^3, as given in Table V. However, when they are pressed into fuel pellets, the entire length of the fuel stack will not be composed of fuel, as there are dishes, gaps, and chamfers applied in the manufacturing process. For the conventional HWR NU fuel pellet design, the combined effects of fuel porosity and gaps between pellets due to pellet geometry are accounted for by scaling the fuel density. These combined effects yield an effective density of the fuel stack of 10.6 g/cm^3 for uranium dioxide. By extension and assuming the same porosity and pellet-to-pellet gaps, the thorium dioxide and plutonium dioxide would be scaled by a similar factor to 9.7 g/cm^3 and 11.1 g/cm^3, respectively [8]. Further scaling is then applied to adjust the densities to smear the axial features into a two dimensional model. This scaling factor is calculated as the nominal fuel stack length (48 cm) divided by the nominal bundle length (49.53 cm). The application of the scaling factor results in densities of 10.3 g/cm^3 for uranium dioxide, 10.8 for plutonium dioxide, and 9.4 g/cm^3 for thorium dioxide. The density values are adjusted to allow for margin in the burnup calculations with lower densities for uranium and plutonium of 10.0 g/cm^3 and 9.7 g/cm^3 respectively and a higher thorium density of 9.7 g/cm^3. Using a higher density of 9.7 g/cm^3 for thorium is more conservative, as it will result in a lower value for reactivity and burnup. The approximate densities used are suitable for these scoping studies of various fuel bundle concepts. In actual fuel design or physics validation studies, measured values for densities of UO_2, PuO_2, and ThO_2 would be used in lattice physics calculations.

V. ANALYSIS RESULTS

V.A. 2-D WIMS-AECL Safety/Operational Characteristics

The results of the lattice physics analyses with WIMS-AECL are summarized in Table VII. The CVR is plotted against burnup for each lattice concept in Figure 3. The highest burnup averaged CVR is observed in the NU case. The (Pu,Th) cases have lower CVR than NU. There is a slightly higher burnup-averaged CVR seen in the duplex lattice concepts over homogeneous fuel pellets (~0.2 mk). The (LEU,Th) cases have more distinctive differences in CVR for duplex fuel cases, dropping by 1 mk for duplex fuels. This difference in CVR is likely caused by the large differences in the fuel composition between annuli compared to the plutonium/thorium cases. The (^{233}U,Th) cases show burnup-averaged CVR values that are similar to the low burnup (Pu,Th) lattice concepts studied, again with little difference between duplex and homogeneous fuel pellets.

The burnup-averaged fuel temperature coefficient is given in Table VII and the individual plots for each lattice concept as a function of burnup are shown in Figure 4. NU achieves a burnup-averaged FTC of -0.0022 mk/K and the trend increases with burnup. All other fuel types in the BUNDLE-35 fuel bundle geometry have a more negative FTC. A negative fuel temperature coefficient is a key contributor to the power coefficient of reactivity in a postulated accident scenario involving a power increase. The burnup averaged FTC of the (^{233}U,Th) concepts, approximately -0.0090 mk/K, is close in magnitude to that of the (LEU,Th) concepts. The (Pu,Th) fuels have burnup-averaged FTC values between -0.0055 mk/K and -0.0063 mk/K.

The linear element ratings for each lattice concept and fuel ring are given in Figure 5. For all fuel types, the highest linear element ratings are found in the outermost fuel ring. Some concepts have more evenly distributed power profiles over time. The (^{233}U,Th) concepts, LC-14b and LC-15b, for example, have only a slight variation in element rating as the fuel depletes, which is desirable from an operating perspective. The LER balance in the fuel rings of (^{233}U,Th) fuel is relatively constant for the duration of its residence in the core with ~66%/34% power distribution between the outer/inner fuel rings. The (Pu,Th) fuels show the largest variations, with LERs changing by 10 kW/m in the inner and outer fuel pins over the operating life of the bundle. The power distribution between rings of fuel for (Pu,Th) fuels is the least balanced with 72% of bundle power in the outer ring and 28% in the inner ring for fresh fuel. At exit burnup, the power balance is closer to the (^{233}U,Th) bundle, with ~65%/35% distribution of power across fuel rings. NU fuel in LC-01 has a much smaller change in LER, generally within 1 kW/m, over burnup. At zero burnup, the power is distributed 55% in the outer ring, 30% in the third ring, 13% in the second ring, and 0.02% in the central element. The (LEU,Th) fuels have a smaller range in LER with burnup, compared to (Pu,Th), with ~54 kW/m in the outer ring and ~40 kW/m in the inner ring for fresh fuel, and 51 kW/m and 43 kW/m at exit burnup. The power distribution in the (LEU,Th) fuel is 66%/34% for fresh fuel. The maximum LER values per bundle for an 800 kW bundle are given in Table VII. The highest LERs are seen in the (Pu,Th) fuel. The low burnup (LEU,Th) and (^{233}U,Th) exhibit very similar maximum LERs, between 52 and 53 kW/m, only slightly higher than the NU maximum LER of 51 kW/m.

Table VII
Lattice Analysis Results

Lattice Concept	Burnup Average CVR (mk)	Burnup Average FTC (mk/K)	Maximum LER(1) (kW/m)	Burnup Average CR (-)	FIR @ Exit Burnup (-)	Relative Fissile Utilization(2) (-)	Lattice Estimated Exit Burnup (MWd/tiHE)
LC-01	14.01	-0.0022	51.48	0.77	0.71	0.95	7,104
			Plutonium/Thorium				
LC-06b	8.39	-0.0054	57.37	0.76	0.63	0.99	23,636
LC-07b	8.50	-0.0053	57.51	0.76	0.62	0.99	23,636
LC-08b	9.33	-0.0063	58.93	0.75	0.52	1.21	37,166
LC-09b	9.49	-0.0063	59.09	0.75	0.52	1.21	37,396
			LEU/Thorium				
LC-10b	10.80	-0.0099	52.87	0.77	0.64	1.20	24,358
LC-11b	9.90	-0.0094	52.97	0.76	0.58	1.31	26,877
LC-12b	10.96	-0.0088	53.47	0.74	0.44	1.60	40,643
LC-13b	9.78	-0.0081	53.57	0.71	0.39	1.60	41,091
			^{233}U/Thorium				
LC-14b	8.59	-0.0091	52.46	0.92	0.90	0.99	18,279
LC-15b	8.57	-0.0087	52.54	0.91	0.89	1.03	18,969

(1) LER assuming a maximum bundle power of 800 kW.
(2) Relative Fissile Utilization is that normalized against nominal fissile utilization for a large PT-HWR operating with natural uranium fuel, which is approximately 1,056,000 MWd/t-fiss (7,500 MWd/t / 0.0071).

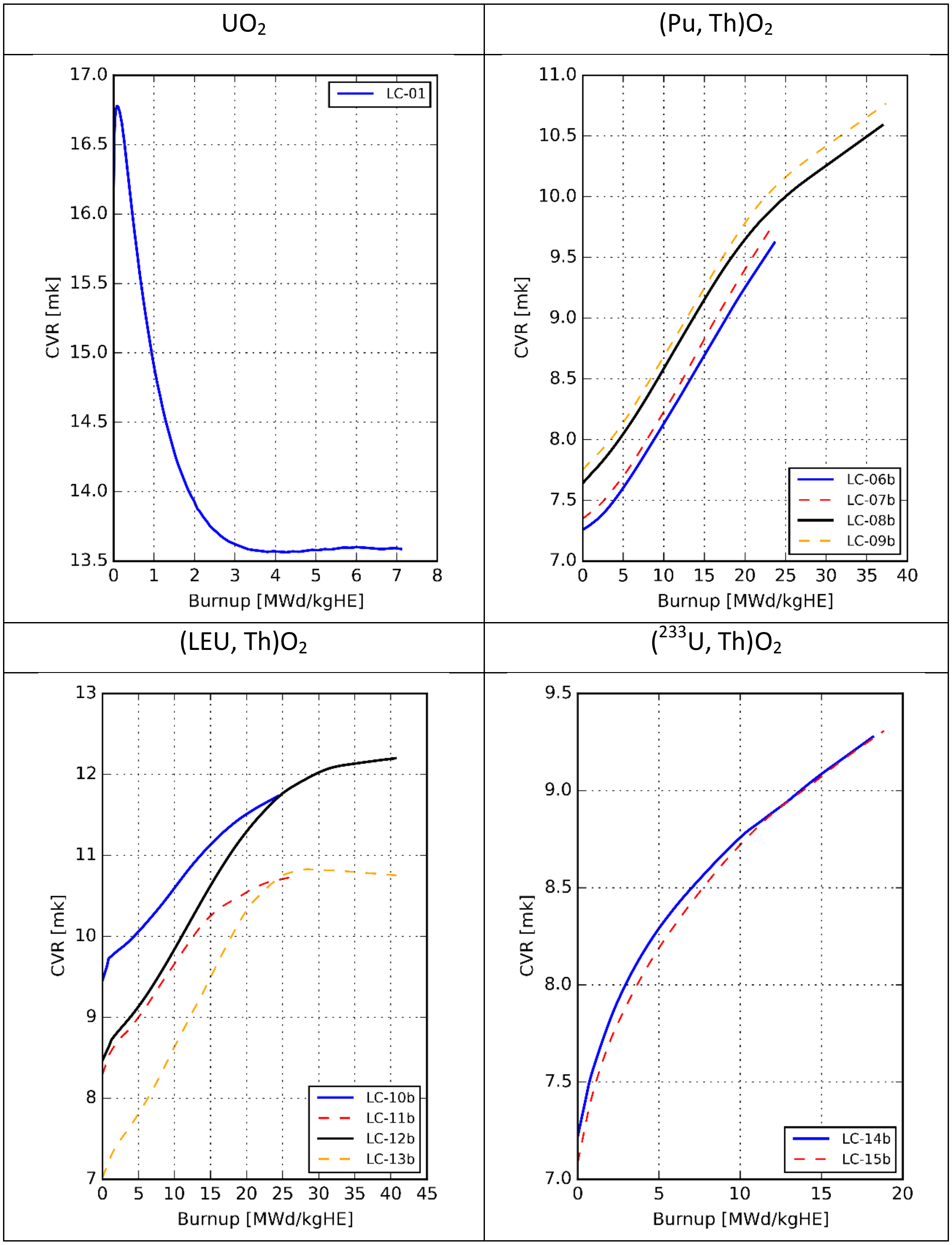

Figure 3: CVR as a Function of Burnup for the Fuel Concepts Studied

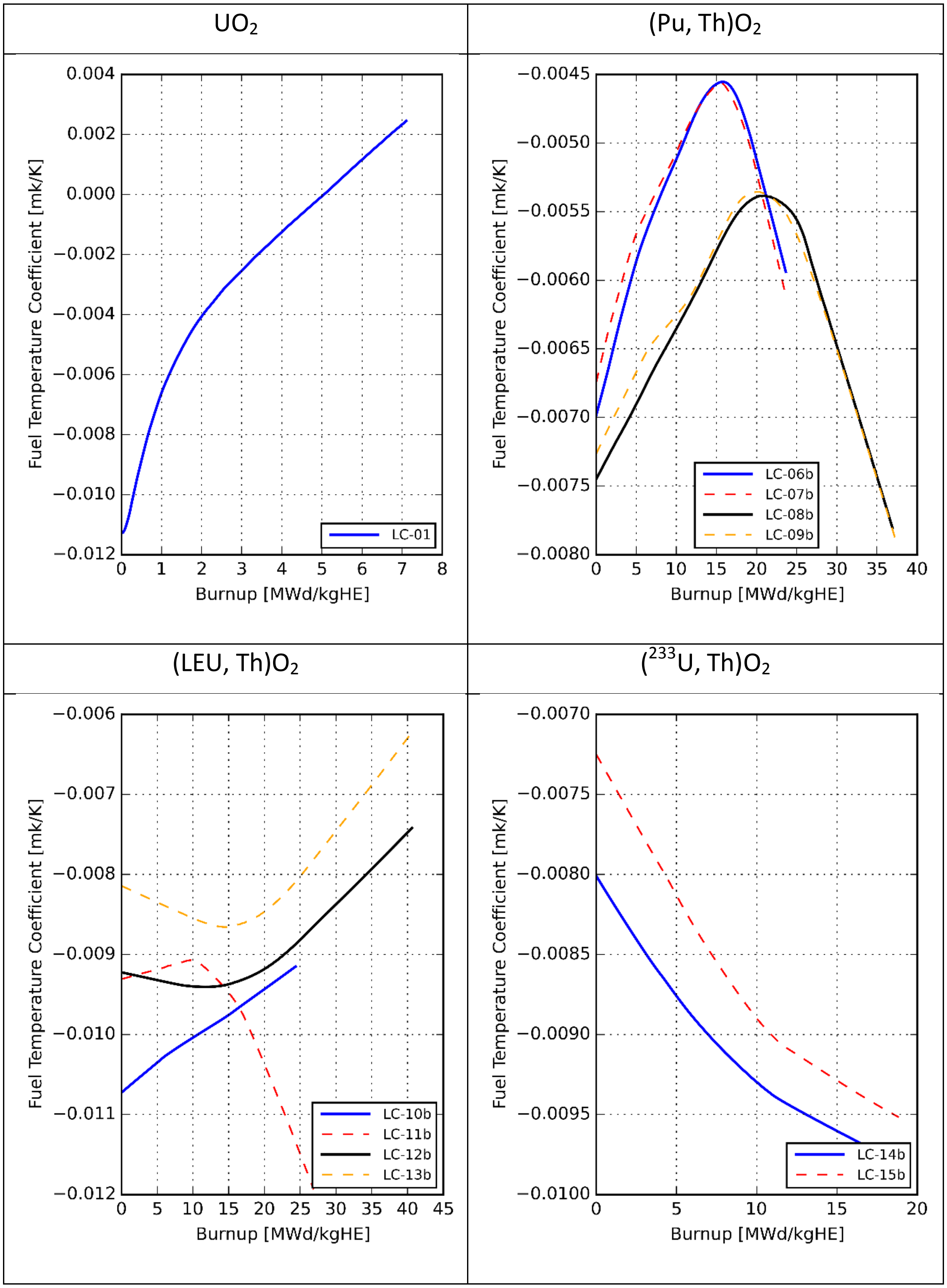

Figure 4: Fuel Temperature Coefficient as a Function of Burnup for the Fuel Concepts Studied

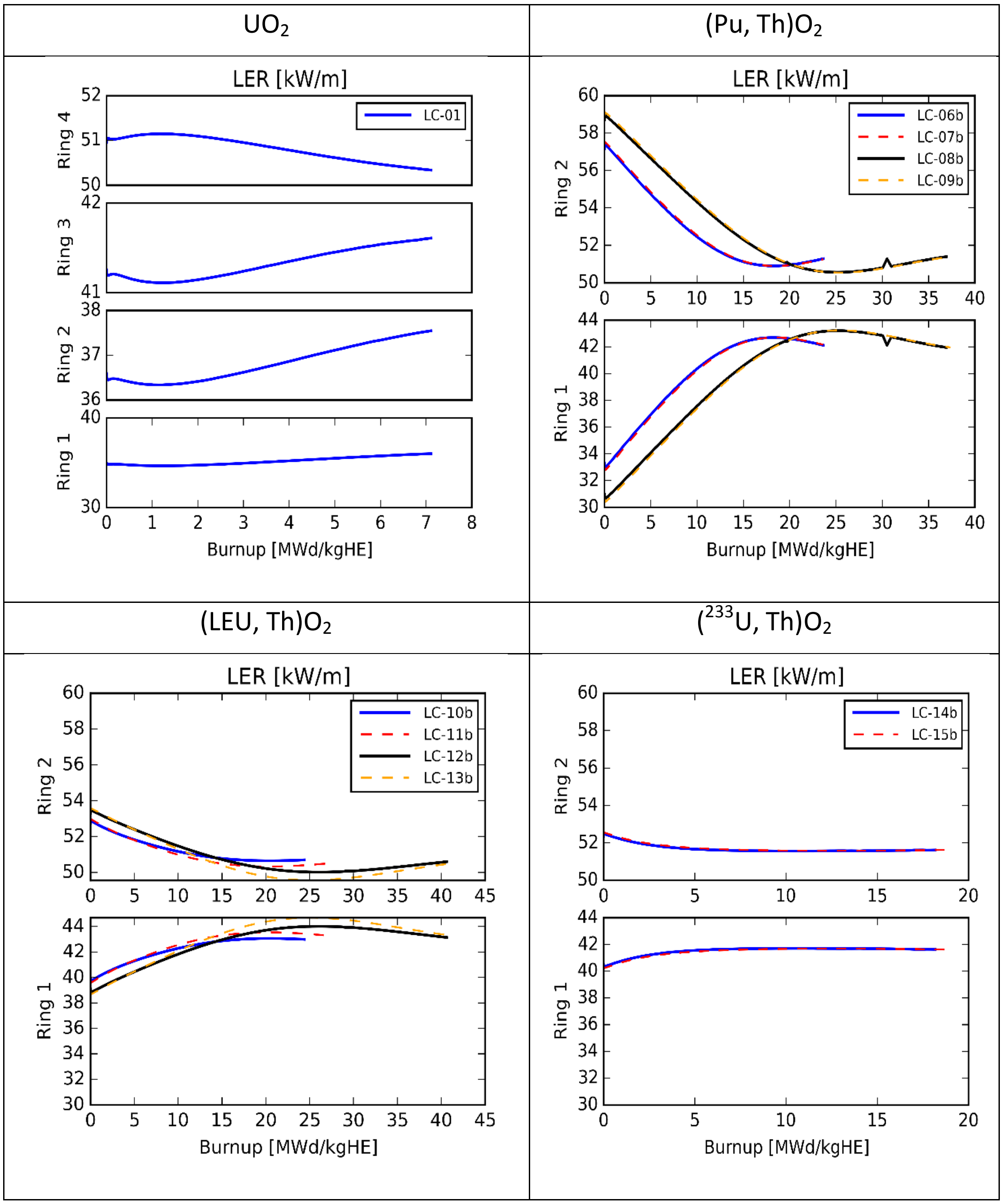

Figure 5: Linear Element Rating as a Function of Burnup for the Fuel Concepts Studied

V.B. WIMS-AECL 2-D Performance Characteristics

Plots of k-infinity vs. burnup for each fuel bundle concept are shown in Figure 6. The exit burnup values were estimated for each lattice concept and are given in Table VII. The (Pu,Th) and (^{233}U,Th) Duplex fuels behave similarly to the homogeneous fuels (Duplex fuels are shown with dotted lines in the figure). The (LEU,Th) fuel k-infinity curve is noticibly steeper for Duplex fuel compared to homogeneous fuel. The postulated reason for this is the significant difference in fuel composition across the fuel pellet with 100% LEU in the outer fuel annulus and 100% thorium in the inner annulus. The (LEU,Th) bundles have exit burnup values in a similar range, between 24.3 – 41.1 MWd/kgHE, with distinctively higher exit burnups for the Duplex concepts. The other fuel types don't show significant differences in exit burnup between the Duplex and homogeneous fuel elements.

The conversion ratio as a function of burnup is shown in Figure 7, with the burnup-averaged conversion ratio provided in Table VII. The behavior of the conversion ratio as the fuel is depleted differs significantly between NU and the mixed oxide thorium-based fuels. The NU conversion ratio has a 'U' shaped curve, initially decreasing with burnup and then increasing at 2.5 MWd/kgHE. All of the mixed oxide thorium-based fuels trend towards an increasing CR with burnup. The (Pu,Th) fuels achieve a CR greater than 1 (making more fissile material than consuming) by the time they reach exit burnup.

The fissile inventory ratio as a function of burnup is shown in Figure 8. Natural uranium fuel has an FIR that constantly decreases with burnup since it is losing fissile material at a constant rate relative to the initial fissile material it contains. The other fuel types show a tapering FIR, indicating that significant breeding of fissile material is occurring to slow the rate of loss. In the context of once-through cycles, it can be desirable to have a low FIR at exit burnup to show that most of the initial fissile material was used. With (^{233}U,Th) fuels, however, a higher FIR is desirable, to indicate that significant breeding of ^{233}U has occurred during depletion. The LC-14b and LC-15b concepts’ FIR of approximately 0.9 is therefore very encouraging.

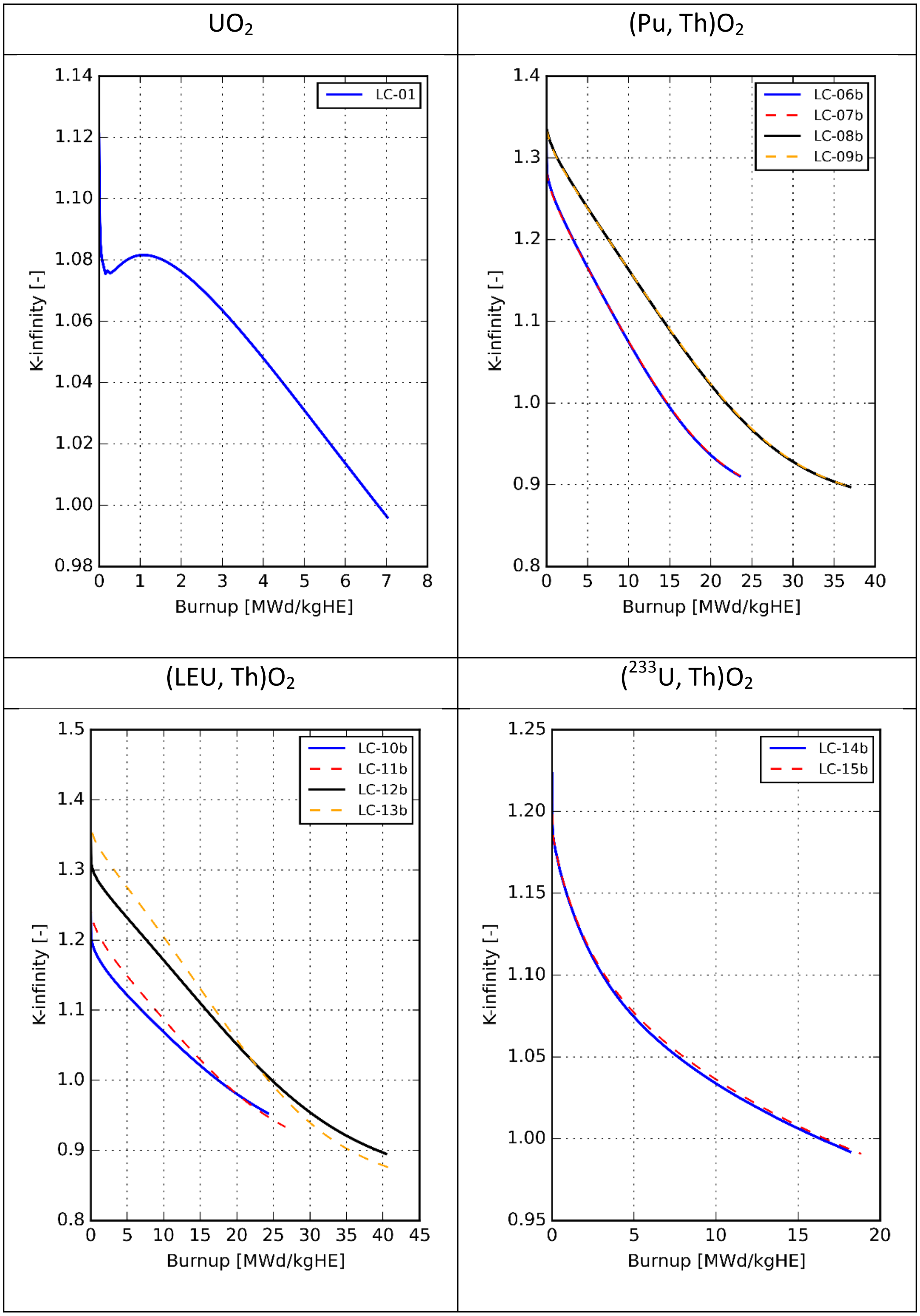

Figure 6: k-infinity as a Function of Burnup for the Fuel Concepts Studied

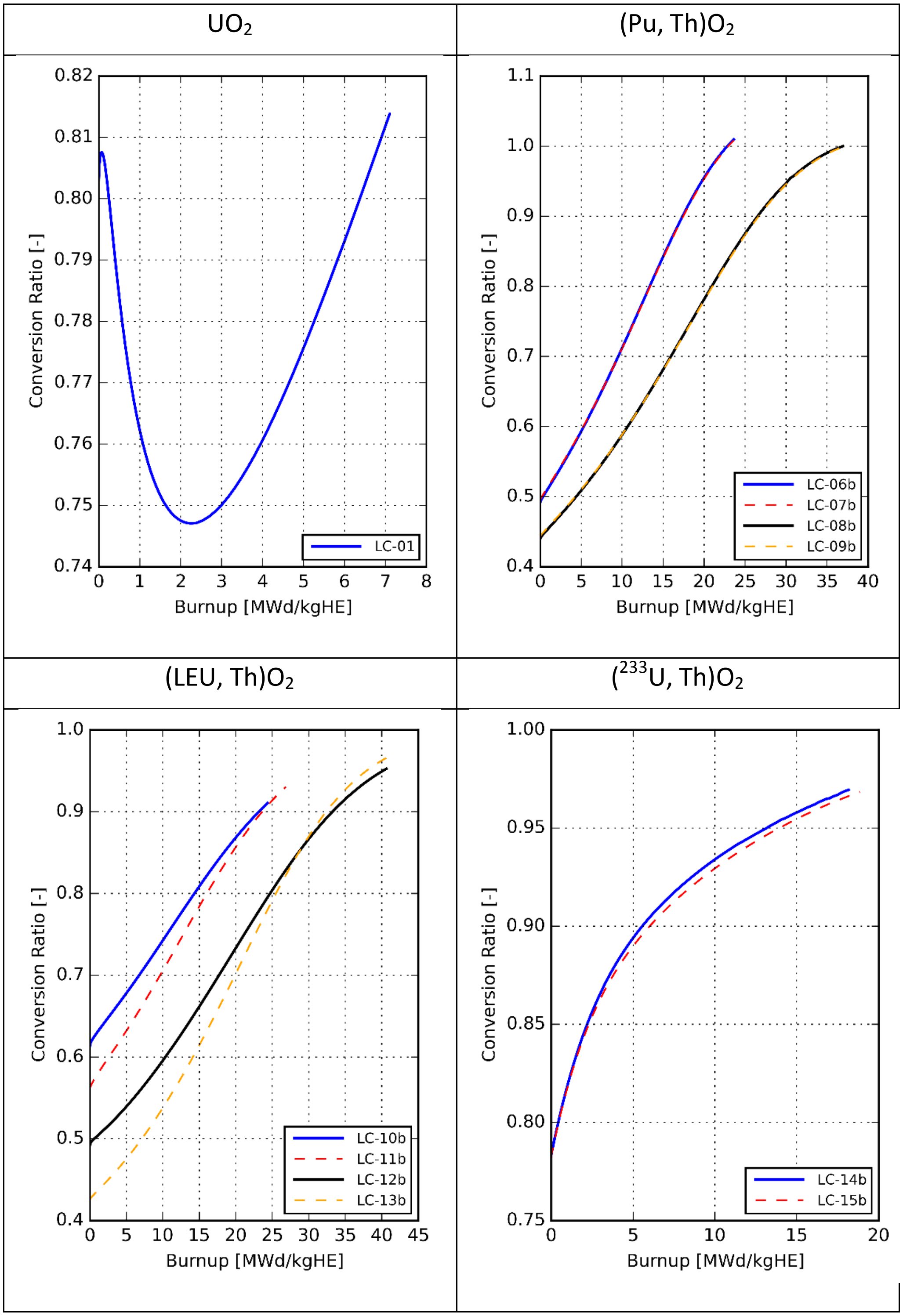

Figure 7: Conversion Ratio as a Function of Burnup for the Fuel Concepts Studied

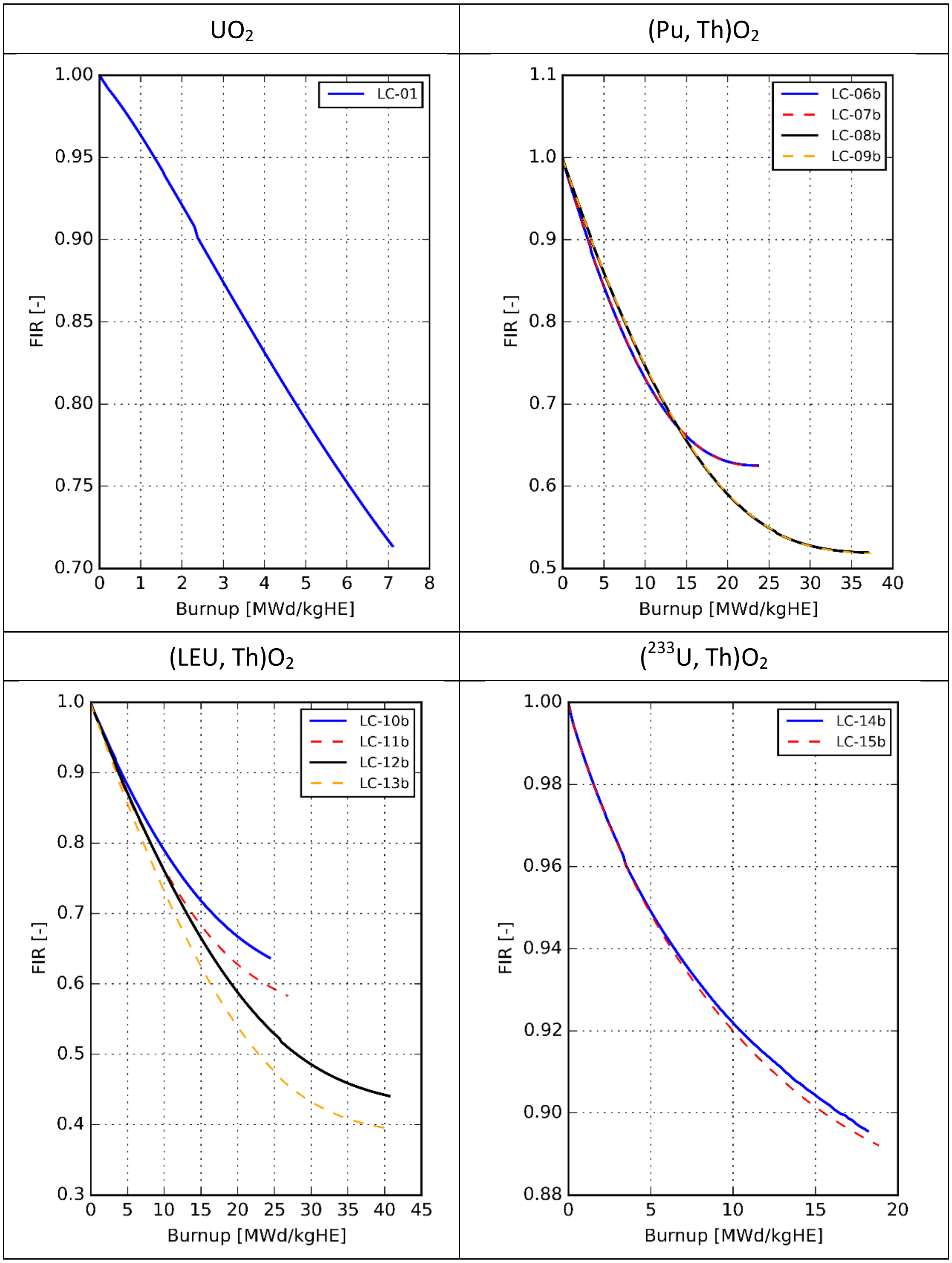

Figure 8: Fissile Inventory Ratio as a Function of Burnup for the Fuel Concepts Studied

The mass of fissile nuclides (^{235}U, ^{239}Pu, ^{241}Pu, and ^{233}U) in the fuel bundle for fresh and exit burnup are given in Table VIII. The (Pu,Th) fuel produces the most ^{233}U at exit burnup with 136 – 159 g/bundle. It should be noted that most of the initial fissile plutonium is actually burned by the time the bundle reaches discharge burnup, with approximately only 40 grams of the initial 290-390 grams of fissile plutonium remaining. If dispositioning reactor grade plutonium is a desired outcome, these lattice concepts would efficiently reduce the mass of plutonium down to 16% of the initial amount for the lower burnup concepts (LC-06b and LC-07b) or down to 9% for the higher burnup lattice concepts (LC-08b and LC-09b). The (LEU,Th) fuels consume almost all of the initial fissile ^{235}U (14%-3% of original amount remains), and breed about 100 grams of ^{233}U. Small amounts of fissile plutonium are produced, though most of it is burned in situ with about 20 grams remaining at exit burnup. The amount of ^{233}U initially required for the (^{233}U,Th) concepts is about 227 grams/bundle. Over the course of depletion, only a net 27 grams of ^{233}U are lost.

The net fissile nuclide production per bundle is given in Table IX. This Table includes a new metric termed fissile efficiency (FE), calculated as the burnup (MWd/kgHE) multiplied by the initial mass of heavy element (kgIHE) and divided by the net fissile material used per bundle (MWd/g fissile consumed). This metric measures the amount of power obtained relative to the amount of fissile fuel consumed. Fissile efficiency is a slightly different evaluation metric than fissile utilization because it relates to the fissile material used in comparison to the fissile material initially required, and therefore more adequately represents the effectiveness of highly breeding (^{233}U,Th) fuels. The fissile efficiency for NU, at 3.27 MWd/g fissile consumed, is actually quite close to the (LEU,Th) and (Pu,Th) fuel types. The low burnup LEU cases outperform NU at using fissile material to produce power. Conversely, the (^{233}U,Th) fuels show excellent use of fissile material relative to power produced by the bundle with a fissile efficiency of 10 MWd/g fissile consumed, three times higher than natural uranium.

Table VIII
Grams of Fissile Materials Produced/Consumed Per Bundle

Lattice Concept	Final Amount				Initial Amount				Net Amount Produced/Used			
	^{233}U*	^{235}U	^{241}Pu	^{239}Pu	^{233}U*	^{235}U	^{241}Pu	^{239}Pu	^{233}U*	^{235}U	^{241}Pu	^{239}Pu
NUO_2												
LC-01	0.00	42.93	3.98	46.39	0.00	134.40	0.00	0.00	0.00	-91.46	3.98	46.39
$PuO_2 + ThO_2$												
LC-06b	136.87	0.94	27.15	19.68	0.00	0.00	66.93	228.33	136.87	0.94	-39.78	-208.65
LC-07b	136.70	0.94	27.10	19.64	0.00	0.00	66.93	228.32	136.70	0.94	-39.84	-208.68
LC-08b	159.25	1.93	25.83	10.07	0.00	0.00	86.06	293.58	159.25	1.93	-60.23	-283.51
LC-09b	159.98	2.00	25.29	9.48	0.00	0.00	86.06	293.57	159.98	2.00	-60.76	-284.10
$LEUO_2 + ThO_2$												
LC-10b	106.81	35.44	3.06	15.62	0.00	253.92	0.00	0.00	106.81	-218.48	3.06	15.62
LC-11b	109.26	24.31	2.78	12.48	0.00	257.03	0.00	0.00	109.26	-232.72	2.78	12.48
LC-12b	101.66	14.44	4.69	18.51	0.00	318.38	0.00	0.00	101.66	-303.94	4.69	18.51
LC-13b	96.50	10.61	3.97	15.32	0.00	323.29	0.00	0.00	96.50	-312.68	3.97	15.32
$^{233}UO_2 + ThO_2$												
LC-14b	200.79	2.69	0.00	0.00	227.35	0.00	0.00	0.00	-26.56	2.69	0.00	0.00
LC-15b	199.98	2.81	0.00	0.00	227.45	0.00	0.00	0.00	-27.47	2.81	0.00	0.00

*The calculated mass of ^{233}U also includes the mass of ^{233}Pa.

Table IX
Net Fissile Material Consumed per Bundle (grams) and Total Power Produced per Gram of Net Fissile Material Consumed per Bundle

Lattice Concept	Net Fissile (grams)	Fissile Efficiency (MWd/g Fissile Consumed)
LC-01	-41.10	3.27
LC-06b	-110.63	2.79
LC-07b	-110.88	2.78
LC-08b	-182.55	2.66
LC-09b	-182.88	2.66
LC-10b	-92.98	3.46
LC-11b	-108.20	3.28
LC-12b	-179.08	3.01
LC-13b	-196.89	2.77
LC-14b	-23.87	10.00
LC-15b	-24.66	10.04

VI. SUMMARY AND CONCLUSIONS

Possible options for introducing thorium-based mixed oxide fuels into the PT-HWR fuel cycle were evaluated with 2-D lattice physics depletion analysis using the transport code WIMS-AECL.

The fuel compositions studied were natural uranium, plutonium/thorium, LEU/thorium and ^{233}U/thorium. The NU fuel was modelled in a 37-element bundle geometry and used as a baseline for comparison. All of the mixed oxide fuels studied were modelled in a 35-element bundle geometry with a large central graphite moderator/displacer surrounded by two rings of fuel.

Based on the WIMS-AECL 2-D analysis, some key conclusions can be made. First, all thorium based concepts studied here can result in lower (though still small in magnitude) fuel temperature coefficients and lower coolant void reactivity values (~4-5 mk lower) relative to the natural uranium bundle. Of the eight lattice concepts studied with the intent of producing ^{233}U for later use (LC-06b to LC-13b), the low burnup (LEU,Th) option (LC-10b) is most suiTable for use in a PT-HWR. Though (LEU,Th) fuels produce less ^{233}U than (Pu,Th) fuels, they behave more closely to the NU fuel, namely in terms of: the power balance in the fuel bundle, the maximum LER value (52.9 kW/m), and the reactivity swing from fresh – exit burnup fuel (250 mk vs 400 mk for (Pu,Th) fuels). The latter factor makes the fuel less likely to cause high bundle power transients during refueling operations. The (LEU,Th) concepts also have the highest fissile utilization (relative to NU), indicating the most burnup is obtained relative to the initial fissile material present, with values near 1.3 and 1.6 for the low and high burnup options.

The (^{233}U,Th) concepts are most attractive in terms of bundle power balance. Not only do these fuels have comparable maximum LERs to the natural uranium bundle (52.5 kW/m vs. 51.5 kW/m), but they also have a very small variation in the power balance in the bundle during the course of depletion.

The 'fissile efficiency' was introduced in this work as a new metric, defined as the amount of power obtained from a bundle multiplied by the residence time and divided by the net fissile material consumed. It was shown that by this metric, the fuels most efficient at using fissile material to produce power are the highly breeding (^{233}U,Th) lattice concepts. These have fuel efficiencies of about 10 MWd/g, in comparison to 3.2 MWd/g for natural uranium. Values near 3 MWd/g are achieved for all other lattice concepts.

The (Pu,Th) concepts were able to breed the most ^{233}U, with 140-160 g produced per bundle at discharge burnup, showing greater breeding advantage than the (LEU,Th) fuels which produced approximately 100 g/bundle. However, the reprocessing of reactor grade plutonium for fuel fabrication, the performance burden of higher linear element ratings, and a larger reactivity swing in the bundle represent added costs of (Pu,Th) fuels that must be considered. A reduction in the total reactor power may be required during the full core analysis of the (Pu,Th) concepts due to the significantly higher linear element ratings. Despite these drawbacks, it is worthwhile to further investigate this set of (Pu,Th) lattice concepts because of their efficacy in dispositioning fissile plutonium.

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