

# Lattice physics evaluation of 35-element 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 calculations with depletion were carried with WIMS-AECL Version 3.1 out as part of exploratory scoping studies to evaluate various thorium-based fuel bundle concepts for potential application in pressure tube heavy water reactors (PT-HWRs). Fuel bundles concepts investigated consisted of a cluster of 35 fuel elements arranged in two rings (14 + 21), and surrounding a central graphite displacer rod. The fuel is comprised of thorium dioxide mixed with a fissile driver of reactor-grade plutonium (~67 wt% Pu<sub>fissile</sub>/Pu; 3.5–4.5 wt% PuO<sub>2</sub>/(Pu,Th)O<sub>2</sub>), low enriched uranium (5 wt% <sup>235</sup>U/U; 40–50 wt% LEUO<sub>2</sub>/(LEU,Th)O<sub>2</sub>) or uranium-233 (1.8 wt% <sup>233</sup>UO<sub>2</sub>/(<sup>233</sup>U,Th)O<sub>2</sub>). Estimates of burnup-averaged fuel temperature coefficients (FTC) and coolant void reactivity (CVR) were found to be lower than those for conventional natural uranium dioxide (NUO<sub>2</sub>) PT-HWR fuel in a 37-element bundle. A low-burnup option for using (LEU,Th)O<sub>2</sub> fuel in a PT-HWR is found to be attractive as a means for extracting energy from thorium, while also generating stockpiles of <sup>233</sup>U, and demonstrating enhanced safety characteristics with reduced CVR and FTC relative to NUO<sub>2</sub>.

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## 1. Introduction

As a fertile nuclear fuel that is nearly three times as abundant as uranium (OECD, 2014), 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 conventional light water reactors and other types of reactors. For example, see references by Galperin (2002), IAEA (2005), Todosow (2005), Yun (2010), Bjork (2013), OECD (2015), Ade (2016), and Ault (2017). However, the opportunities and potential advantages for using thorium-based fuels in pressure tube heavy water reactors (PT-HWR) may be even greater. The use of thorium-based fuels in PT-HWRs has been a topic of in-depth study for many decades, including past work, for example by Lewis (1947), IAEA (1979), Milgram (1982), and Milgram (1984), and more recent studies, as shown in references by Boczar (2002), Mao (2009), Ovanes (2012), Bromley (2014), Bromley (2016a), Bromley (2016b), Bromley (2016c), Bromley (2017), Colton (2016), Colton (2017a), and Colton (2017b). 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 (IAEA, 1979; Griffiths, 1983; IAEA, 2002).

In previous lattice physics studies (Bromley, 2014), several different bundle concepts were assessed for using thorium-based fuels in PT-HWRs. From those studies, it was found that a 35-element bundle with a central displacer rod made of ZrO<sub>2</sub> was good compromise for achieving high fuel burnup and high fissile utilization, while also maintaining a low CVR. Subsequent studies by Bromley (2016a,b) assessed the impact of power levels and power histories for lower fissile content thorium-based fuels (3 wt% Pu/(Pu + Th) and 1.7 wt% <sup>233</sup>U/(U + Th)) with ZrO<sub>2</sub> displacer rods, and it was found that the use of an assumed bundle power of ~600 kW for lattice physics burnup calculations, and a leakage reactivity margin of 35 mk (1 mk = 100 pcm = 0.001 Δk/k) would give a slightly conservative lower estimate of the achievable burnup of thorium-based fuels in a PT-HWR. Later investigations of these same lattices and pure ThO<sub>2</sub> blanket-type lattices (Bromley, 2016c, 2017), assessed the impact of modifications to the heavy water purity, zirconium enrichment, alternative fuel management schemes, and moderator-to-fuel ratio on the performance and safety characteristics and the production of <sup>233</sup>U. It was found that zirconium enrichment could increase achievable burnup by more

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than 30% for  $\text{NUO}_2$  and  $(^{233}\text{U,Th})\text{O}_2$  fuels, while raising heavy water coolant purity could reduce CVR by at least 0.5 mk. Investigations by Colton, (2016a, 2017a) examined the performance and safety characteristics of uranium-based fuels augmented by small amounts of thorium for potential near-term application in PT-HWRs. This was later followed by code-to-code comparisons benchmarking WIMS-AECL 3.1 (Altiparmakov, 2008) calculations with MCNP (X-5 Monte Carlo Team, 2005) calculations for both uranium-based fuels and several thorium-based fuels with solid homogeneous fuel pellets (Colton, 2017b).

In the current work, two-dimensional lattice physics calculations were performed with WIMS-AECL 3.1 for a number of thorium-based fuel bundle concepts in a 35-element bundle geometry for potential application in PT-HWRs. These bundle concepts included both homogeneous fuel pellets, and radially-heterogeneous fuel pellets (duplex fuel). From the lattice physics calculations, various performance and safety characteristics were estimated, including the conversion ratio (CR), the fissile inventory ratio (FIR), the exit burnup (BU-exit), the individual fissile isotope content, and the fissile utilization (FU). The key operations and safety parameters that were estimated include the coolant void reactivity (CVR), fuel temperature coefficient (FTC), and the maximum linear element rating (LER). The results obtained were compared against those obtained earlier for conventional natural uranium fuel in a 37-element fuel bundle geometry (Colton, 2017a).

## 2. Pressure Tube heavy water reactors and lattice concepts

PT-HWRs differ from pressurized water reactors (PWRs) and boiling water reactors (BWRs) in that PT-HWRs use an array of parallel pressure tubes, each containing an individual fuel assembly (or string of short, individual fuel bundles) instead of one large pressure vessel. Details about PT-HWR and their operational characteristics can be found in other works (IAEA, 2002; Griffiths, 1983). In this study, the structural components of the fuel channel are similar to currently operating PT-HWRs (IAEA, 2002; Marleau, 2008). Modelling parameters including temperatures, dimensions and materials for the various lattice components can be found in Tables 1 and 2.

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 Fig. 1.

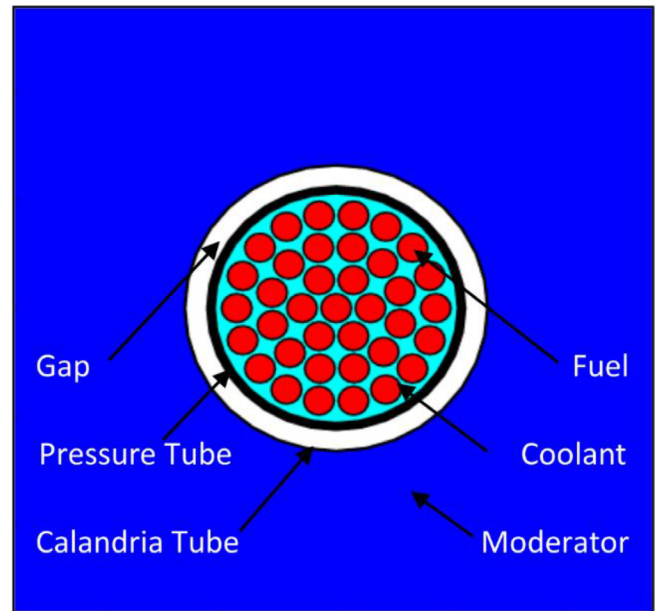
The other fuel assembly studied is the BUNDLE-35 concept, consisting of two rings of fuel elements (21 outer pins + 14 inner pins) as shown in Fig. 2. The BUNDLE-35 geometry has similarities to 43-element bundles studied previously (Boczar, 2002; Mao, 2009; Bromley, 2014), but the central 8 fuel elements (7 inner-inner pins + 1 central pin) are replaced with a central displacer rod made of a low-neutron-absorbing material, such as graphite.

Two types of fuel pellet geometry were studied in this fuel bundle type: homogeneous pellets (Fig. 2(a)) and duplex-type heterogeneous pellets (Fig. 2(b)). The duplex fuel elements consist of an inner pure  $\text{ThO}_2$  pellet, surrounded by outer annular pellet the

**Table 2**  
Nominal material specifications (Marleau, 2008).

Structure	Temp.(K)	Material	Density (g/cm <sup>3</sup> )
Coolant	561	99.1 wt% D <sub>2</sub> O	0.81
Pressure Tube	561	Zr-2.5Nb	6.52
PT/CT Gap	451	<sup>12</sup> CO <sub>2</sub>	0.0012
Calandria Tube	342	Zircaloy-2	6.54
Moderator	342	99.7 wt% D <sub>2</sub> O	1.09

\*CO<sub>2</sub> is used in the gap because of its low neutron capture cross section. Alternative gases such as N<sub>2</sub> or air are avoided since the radiation field may cause ionization and the formation of NOX compounds.



**Fig. 1.** BUNDLE-37 (B37) Geometry.

containing fissile fuel, in the form of  $(\text{Pu,Th})\text{O}_2$ ,  $(\text{LEU,Th})\text{O}_2$ , or  $(^{233}\text{U,Th})\text{O}_2$ , as illustrated also in Fig. 3. The fraction of fissile fuel in the outer annulus of the duplex fuel is higher (2–2.5 times higher) than what would be found in the homogeneous fuel pellets, given that the inner pellet is 50% to 60% of the total pellet volume. There are a number of potential advantages of using duplex fuel. The first is that in the initial stages of burnup, when the fuel has a higher level of reactivity, and higher power levels, the power generation will occur mainly in the outer annular pellet, closer to the outer heat transfer surface (the clad) and the coolant. Thus, heat transfer to the coolant will be enhanced, and the pellet-averaged fuel temperature will be reduced, which should help reduce the probability of fission product migration and potential fuel failures. Another potential advantage is that the irradiated  $\text{ThO}_2$  inner pellet could be easier to reprocess and recycle for extracting  $^{233}\text{U}$ . This feature would be particularly important for  $(\text{LEU,Th})\text{O}_2$  and  $(\text{Pu,Th})\text{O}_2$  fuels, since any  $^{233}\text{U}$  bred in these fuels would be denatured or contaminated by the presence of  $^{238}\text{U}$  or Pu in homogeneous pellets. Previous studies have investigated the feasibility of using duplex-type fuels in light water reactors (LWRs) (Herring, 2001; Zhao, 2001), and significant progress was made in the early 1980s in both manufacturing and irradiation testing prototype duplex-type fuels for potential implementation in LWRs, including thermal breeders (Allen, 1982; Waldman, 1982; Ainscough, 1983; Hoffman, 1982).

The purpose of using a central graphite displacer rod is to reduce the CVR relative to the situation if central fuel elements were used instead. The use of a non-fuel displacer rod instead of

**Table 1**  
Nominal lattice dimensions (Marleau, 2008).

Dimension	Value (cm)
Lattice pitch	28.58
Pressure Tube Inner Radius	5.17
Pressure Tube Outer Radius	5.60
Calandria Tube Inner Radius	6.45
Calandria Tube Outer Radius	6.59

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