Annals of Nuclear Energy 103 (2017) 194-203

Contents lists available at ScienceDirect

Annals of Nuclear Energy

journal homepage: www.elsevier.com/locate/anucene

## Code-to-code comparisons of lattice physics calculations for thoriumaugmented and thorium-based fuels in pressure tube heavy water reactors

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#### ARTICLE INFO

Article history: Received 11 August 2016 Received in revised form 15 January 2017 Accepted 18 January 2017

Keywords: Lattice physics Heavy water reactors Code-to-code comparisons Advanced fuels Thorium

#### ABSTRACT

Code-to-code comparisons of lattice physics calculations were made for a series of fuels that could potentially be used in a conventional 700-MWe class pressure tube heavy water reactor to improve the sustainability of the fuel cycle. Studies were performed for natural uranium, slightly enriched uranium and thorium-based fuels containing low enriched uranium, reactor grade plutonium, or <sup>233</sup>UO<sub>2</sub> as the initial fissile driver. The collision probabilities lattice code WIMS-AECL was compared to the stochastic code MCNP using the ENDF/B-VII.0 nuclear data library. Specific parameters that were studied between models include k-infinity, coolant void reactivity, 89-group cell averaged fluence, and ring-by-ring linear element ratings. The calculations performed have demonstrated that physics parameters estimated by WIMS-AECL are consistent with MCNP, especially for fuel where the main fissile component is uranium-based.

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#### 1. Introduction

Thorium, a fertile nuclear fuel which is nearly three times as abundant as uranium, represents a long-term energy source that could complement uranium and eventually replace it, leading to sustainable energy production (OECD Nuclear Energy Agency and the International Atomic Energy Agency, 2014). An initiative is underway at the Canadian Nuclear Laboratories in Chalk River, Ontario to examine and close the gaps that exist between current science and engineering capability and the potential implementation of thorium-based fuels in conventional, operational pressure tube heavy water reactors (PT-HWRs).

A number of fuel types are under investigation as possible short-term and long-term options for incorporating thorium into the fuel cycle of a pressure tube heavy water reactor. The fuel compositions considered range from natural uranium (as a reference case) to mixed oxide fuels composed mostly of thorium dioxide supplemented with a fissile component in the form of either low enriched uranium (5 wt%  $^{235}$ U/U), reactor grade plutonium or  $^{233}$ U. It is expected that the low enriched uranium could be

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http://dx.doi.org/10.1016/j.anucene.2017.01.023

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obtained from existing enrichment facilities, the reactor-grade plutonium (Nakahara and et al., 2002) could be obtained from stockpiles of spent light water reactor fuel and the <sup>233</sup>U could be obtained from a future stockpile of spent thorium-based fuels (Bromley, 2013).

In a previous study (Colton and Bromley, 2016), full core physics calculations were performed using the neutron diffusion code RFSP (Rouben, 2002) for a number of uranium-based test fuels augmented with thorium in a PT-HWR core. The effects of leakage and online refuelling were modelled in RFSP and key physics parameters such as the full core average burnup, refuelling rates, the maximum bundle and channel powers, and the power distribution were evaluated.

To obtain irradiated fuel compositions, WIMS-AECL (Altiparmakov, 2008) is used to perform lattice-level collision probabilities based depletion calculations, which are homogenized into two group macroscopic cross-sections for the full core RFSP diffusion model. The accuracy of the deterministic core physics calculations with RFSP depends directly on the deterministic lattice physics calculations performed using WIMS-AECL. Therefore, the purpose of this work is to build confidence in lattice physics modeling performed in WIMS-AECL by comparing analogous models built in the continuous energy transport code MCNP (X-5 Monte Carlo Team, 2005) for static material compositions calculated in WIMS-AECL at several burnup steps.





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Abbreviations: PT-HWR, pressure tube heavy water reactor; LC, lattice concept; LER, linear element rating; CVR, coolant void reactivity.

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#### 2. Description of lattice concepts

The lattice concepts described here were modelled with the average operating parameters of a 380-channel 2061  $MW_{th}$  PT-HWR. The two types of fuel bundle geometries studied in this work were a 37-element bundle and a 35-element bundle, as illustrated schematically in Fig. 1a and b, respectively.

The outermost region of the lattice depicts the heavy water  $(D_2O)$  moderator, which is separated from the fuel channel by a Zircaloy-2 calandria tube (Fig. 1a and b). A CO<sub>2</sub> gas annulus separates the calandria tube from the pressure tube, which is composed of Zr-2.5% Nb. The pressure tube contains heavy water coolant and the fuel bundle. The fuel bundle assembly consists of Zircaloy-4 fuel elements, welded together in a cluster formation and filled with oxide fuel pellets. The geometric specifications for the fuel channel and fixed components of the lattice are given in Table 1 and the estimated average operating temperatures and materials of the non-fuel components in this lattice are specified in Table 2. The specific geometric data for the 35-element and 37-element bundles are provided in Table 3. The fuel bundle materials, densities, specific powers and estimated average operating temperatures are given in Table 4.

Six types of fuel were compared in this work; these fuels were mixed with thorium dioxide in different ratios to achieve specific target burnup values. The weight percent composition of each fuel type studied is given in Table 5. The fuel types examined are all in oxide form and include natural uranium (NU), recovered uranium (RU) at 0.95 wt% <sup>235</sup>U/U (recovered from spent light water reactor fuel), slightly enriched uranium (SEU) at 1.2 wt% <sup>235</sup>U/U, low enriched uranium (LEU) at 5 wt% <sup>235</sup>U/U, reactor grade plutonium, and pure <sup>233</sup>U.

Small amounts of thorium (1-2%) by volume) were added to the fuel with the intent of grading the fissile content of the fuel stack horizontally to mitigate end power peaking (Shen, 2001).

In this study we modelled a series of lattice concepts as described in Table 6. The table provides a number of details used to model each concept including the central element material, the outer ring material, the relative power of the bundle, and the total amount of thorium mixed into the end pellets of the fuel specified in length of end pellets.

The 37-element natural uranium fuel bundle (Fig. 1a), with four fuel rings of fuel elements in a cluster geometry, is the standard fuel design used in many operating PT-HWRs. The 35-element

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Geometric specifications for the fuel channel and fixed lattice components.

Geometric description	Value (cm)	
Lattice Pitch	28.6	
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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Average operating temperatures and materials of fuel channel components.

Coolant 561 99.1 wt% D <sub>2</sub> O 0.81   Voided Coolant 561 99.1 wt% D <sub>2</sub> O 0.001   Pressure Tube 561 Zr-2.5% Nb 6.52   Gap 451 CO <sub>2</sub> 0.0012   Calandria Tube 342 Zr-2 6.54   Moderator 342 99.75 wt% D <sub>2</sub> O 1.09	Structure	Temperature (K)	Material	Density (g/cm <sup>3</sup> )
Central Displacer Rod 561 Nuclear Grade Graphite 1.50	Coolant	561	99.1 wt% D <sub>2</sub> O	0.81
	Voided Coolant	561	99.1 wt% D <sub>2</sub> O	0.001
	Pressure Tube	551	Zr-2.5% Nb	6.52
	Gap	451	CO <sub>2</sub>	0.0012
	Calandria Tube	342	Zr-2	6.54
	Moderator	342	99.75 wt% D <sub>2</sub> O	1.09
	Central Displacer Rod	561	Nuclear Grade Graphite	1.50

bundle (Bromley et al., 2016) consists of a central enlarged displacer rod and two outer rings of fuel elements. This bundle is intended for advanced mixed oxide fuel types and is developed to reduce coolant void reactivity by removing the inner fuel rings. Some lattice concepts (LC-07b, LC-11b, LC-13b, LC-15b) are omitted from the table as they belong to fuel bundle configurations that are being assessed at Canadian Nuclear Laboratories, but are not discussed in this work.

#### 3. Analysis methodology

#### 3.1. WIMS-AECL lattice physics analysis

The lattice physics code WIMS-AECL version 3 (Altiparmakov, 2008) is used for depletion calculations. It is a deterministic code that solves the integral form of the neutron transport equation in a fixed number of energy groups using the collision probabilities method. An 89 energy group nuclear data library (Altiparmakov, 2010) based on ENDF/B-VII.0 was used with WIMS-AECL.



Fig. 1. (a) 37-Element lattice cell geometry (left) and (b) 35-element lattice cell geometry (right).

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