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Neutronic Analysis of NaCl-$ThCl_4$-$PuCl_3$ Fuel for Dual-Fluid Reactors †

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Abstract

The neutronic performance of a NaCl-$ThCl_4$-$PuCl_3$ fuel composition for Dual-Fluid Reactors (DFRs) was investigated using the Serpent Monte Carlo code. Different plutonium isotopic compositions were evaluated together with $YH_{1.85}$ moderator and a $ThCl_4$-$PuCl_3$ blanket. The results showed that decreasing the ^{239}Pu content reduced the fuel cycle length in the reference configuration. $YH_{1.85}$ moderator improved thorium utilization and significantly extended the fuel cycle. The proposed blanket further enhanced breeding performance, resulting in fuel cycle lengths exceeding 14,000 effective full-power days (EFPD) for selected cases. Negative fuel temperatureoppler coefficients were maintained throughout the investigated configurations.

Keywords: Dual-Fluid Reactor (DFR); thorium fuel cycle; fast reactor; NaCl-$ThCl_4$-$PuCl_3$ fuel; molten salt reactor; Yttrium Hydride; neutronic analysis; plutonium isotopes; Serpent; fuel cycle length

1. Introduction

The Dual-Fluid Reactor (DFR) is an innovative conceptual reactor design distinguished by its use of two physically separated liquid circuits: a liquid fuel loop and a liquid lead coolant loop [1,2]. The DFR concept is inherently suited for high-temperature operation and is compatible with both chloride-based molten salt fuels (DFRs) and metallic fuels (DFRm). Although substantial research efforts have been devoted to the development of this conceptual reactor, further investigations, especially in the areas of neutronics and fuel cycle performance, are still required.

In this context, the present study focuses on the neutronic characteristics of the DFR concept by proposing a NaCl-$ThCl_4$-$PuCl_3$ fuel salt composition [3,4]. This fuel was selected for its high ^{232}Th content, favorable breeding potential, and lower eutectic temperature than the reference (U-Pu)Cl_3 system [5,6]. Current DFR concepts operate mainly in the epithermal-to-fast spectrum, where high neutron energies can increase material damage and limit reactor lifetime. To mitigate these effects, the incorporation of Yttrium Hydride (YHx) as a moderator has been proposed to enable a thermally moderated DFR design [7,8]. In addition to alleviating material degradation, thermal neutron spectra are known to enhance the utilization efficiency of thorium–plutonium fuel cycles, thereby improving breeding performance and overall neutron economy. Since conventional DFRs operate in an epithermal-to-fast spectrum, $YH_{1.85}$ was introduced to improve thorium utilization and reduce material damage. $YH_{1.85}$ was selected because of its low hydrogen loss at high

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temperatures and demonstrated feasibility in the TCR TCR (The Transformational Challenge Reactor) Program [9,10]. The Serpent Monte Carlo code was used for all neutronic calculations and the ENDF/B-VII.0 cross-section library was used [11,12]. Additionally, in order to facilitate fuel reprocessing, a $ThCl_4$-$PuCl_3$ blanket with different fertile plutonium isotope compositions was proposed to investigate its effect on fuel cycle length. This study investigates (1) the effect of plutonium isotopic composition on DFR fuel cycle length; (2) the impact of the $YH_{1.85}$ moderator; (3) the effect of the $ThCl_4$-$PuCl_3$ blanket; and (4) temperature feedback coefficients for selected cases.

2. Materials and Methods

Lead was used as both coolant and reflector, while SiC was selected as the fuel tube material based on its favorable neutronic performance among SiC, TiC, and ZrC, as well as its commercial availability [13]. The proposed NaCl-$ThCl_4$-$PuCl_3$ fuel has a eutectic point of 597 K with the composition of 0.470 NaCl, 0.354 $ThCl_4$ and 0.176 $PuCl_3$ [3]. The plutonium was assumed to originate from spent VVER-1200 fuel after approximately 10 years of cooling [14], and its isotopic composition was used without modification in the ternary fuel, denoted TF. To investigate the effect of plutonium isotopic composition in DFR, three additional fuels were generated by decreasing the ^{239}Pu content of TF by 10%, 20%, and 60% and adding the reduced amount to ^{240}Pu; These are designated 10TP40, 20TP40, and 60TP40 respectively. Fuel compositions are given in Table 1.

Table 1. Ternary fuel compositions with different plutonium isotope fractions (wt. %).

Isotope	TF	10TP40	20TP40	60TP40
^{232}Th	36.609	36.609	36.609	36.609
^{238}Pu	0.793	0.793	0.793	0.793
^{239}Pu	9.802	8.822	7.842	3.921
^{240}Pu	4.631	5.612	6.592	10.513
^{241}Pu	1.850	1.850	1.850	1.850
^{242}Pu	1.726	1.726	1.726	1.726
Fissile/HM ratio (%)	21.029	19.260	17.491	10.414

YHx was selected as a candidate moderator to investigate its potential for thermalizing the DFR neutron spectrum. Among all YHx compositions, $YH_{1.85}$ was selected since this stoichiometry has proven its feasibility in the TCR program [10,15,16]. A $ThCl_4$–$PuCl_3$ blanket containing only fertile isotopes was also considered to facilitate fuel reprocessing [3,17].

2.1. Serpent Modeling

In this study, the geometry of the 3 GWth Dual-Fluid Reactor was adopted as the reference configuration and modeled using Serpent 1.1.7 with the ENDF/B-VII.0 library [11,12]. The calculations were carried out using 100,000 source neutrons, 100 active cycles, and 50 inactive cycles. The Serpent model of DFRs is shown in Figure 1.

The $YH_{1.85}$ moderator was incorporated by adding 0.05 cm layers between two SiC layers, as this thickness provided the maximum k_{eff} in pin-wise calculations. While increasing the thickness of $YH_{1.85}$, other parameters such as fuel diameter, SiC thickness, pitch length, and fuel volume were kept constant. A geometric representation of this pin configuration is provided in Figure 2.

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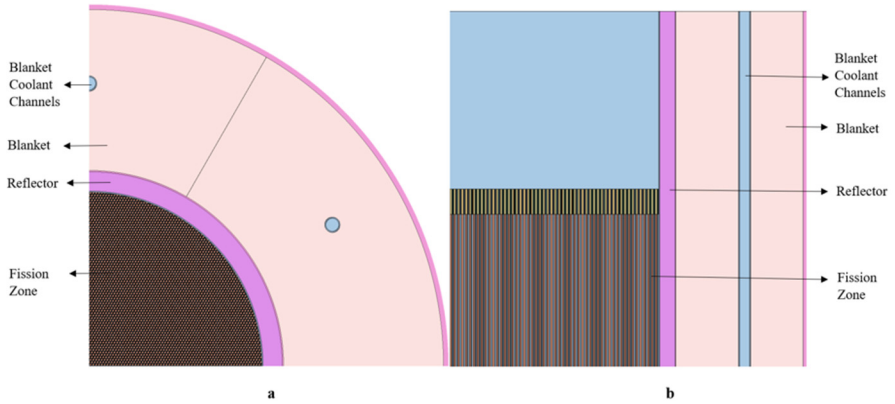


Figure 1. Radial and axial geometries of the DFR: (**a**) radial geometry and (**b**) axial geometry.

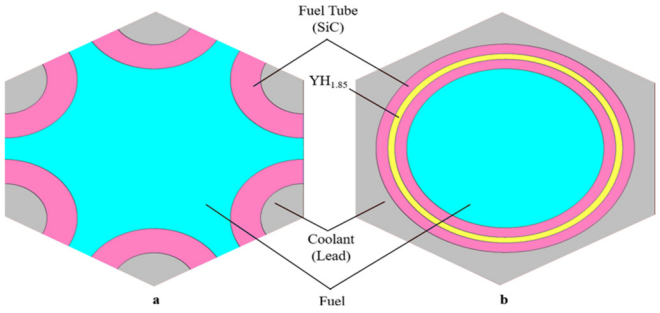


Figure 2. Unit-cell geometries of the fuel channel: (**a**) plenum region and (**b**) core region.

2.2. Reactivity Feedback Evaluation

Reactor safety requires examining how temperature changes affect material behavior and reactivity. To assess this, the fuel temperature coefficient was calculated using Equation (1).

$$\alpha_F = \frac{k_2 - k_1}{k_2 k_1 (T_2 - T_1)}, \quad (1)$$

where α_F is the fuel temperature coefficient; k_1 and k_2 are the effective neutron multiplication factors at temperatures T_1 and T_2, respectively [18,19].

3. Results

Figure 3 presents the variation in k_{eff} with EFPD for different plutonium isotopic compositions in the reference DFR geometry. The TF fuel achieved the longest fuel cycle length among the investigated cases due to its higher fissile plutonium content. As the ^{239}Pu fraction was progressively reduced and replaced with fertile plutonium isotopes, the fuel cycle length decreased significantly.

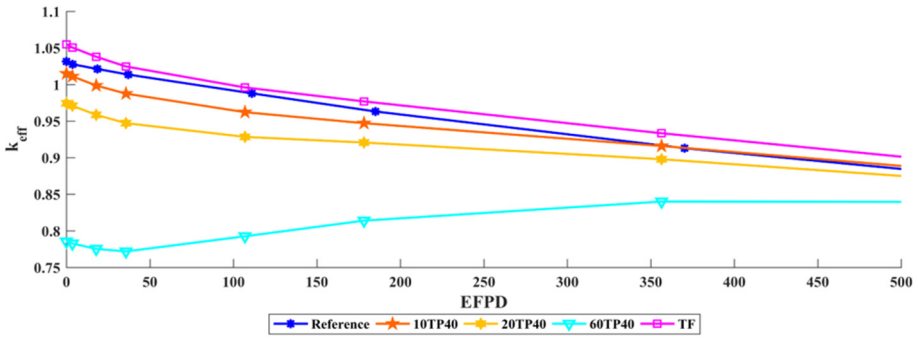


Figure 3. Variation in k_{eff} with EFPD for different fuel compositions in the reference DFR geometry.

Figure 4 shows that $YH_{1.85}$ moderation improved thorium utilization and extended the fuel cycle length.

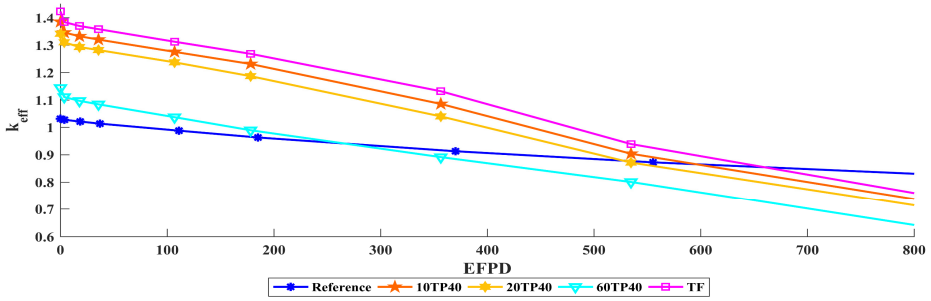


Figure 4. Variation in k_{eff} with EFPD for different fuel compositions in the DFR geometry incorporating a 0.05 cm thick $YH_{1.85}$ moderator layer.

Figure 5 shows that the $ThCl_4$-$PuCl_3$ blanket improved breeding performance and increased fuel cycle lengths to more than 14,000 EFPD. Figure 6 illustrates the combined effect of $YH_{1.85}$ moderation and the $ThCl_4$-$PuCl_3$ blanket. The moderated neutron spectrum enhanced thorium utilization, while the blanket provided an additional source of bred fissile material. Combining the $ThCl_4$-$PuCl_3$ blanket with the $YH_{1.85}$ moderator yielded fuel cycle lengths above 10,000 EFPD, even at relatively low fissile inventories. These findings suggest that the simultaneous use of moderation and thorium-based blanket materials represents a viable option, offering a trade-off between cycle length and material damage.

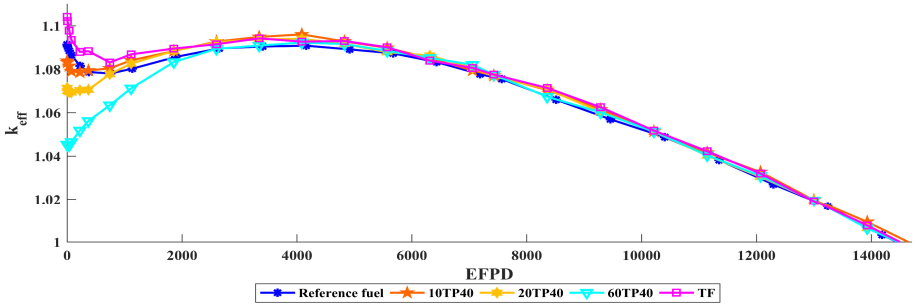


Figure 5. Variation in k_{eff} with EFPD for different fuel compositions using the $ThCl_4$-$PuCl_3$ blanket.

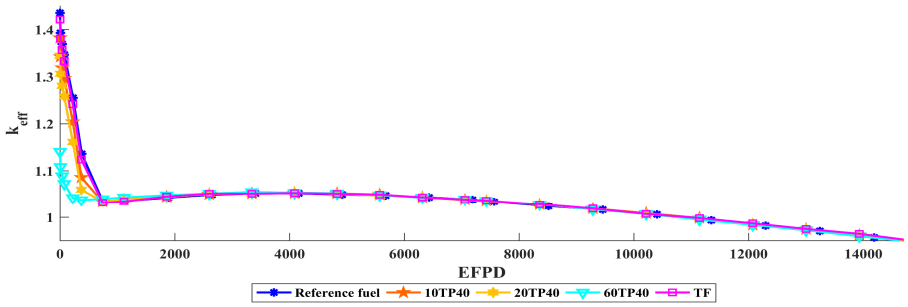


Figure 6. Variation in k_{eff} with EFPD for different fuel compositions using both the $YH_{1.85}$ moderator and the $ThCl_4$-$PuCl_3$ blanket.

Table 2 summarizes the fuel temperatureoppler coefficients and fuel cycle lengths for selected configurations. All investigated cases maintained negative fuel temperature coefficients while achieving substantially longer fuel cycle lengths than the reference DFR design.

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Table 2. Fuel temperature coefficients and fuel cycle lengths for selected configurations.

Fuel	Burnup Stage	α_F (pcm/K) (1100 K–1200 K)	EFPD
Reference	BOC EOC	−40.300 -	75
TF ($SiC/^{238}UCl_3$)	BOC EOC	−9.649 −10.877	97
10TP40 ($SiC/^{238}UCl_3$)	BOC EOC	−10.820 −10.776	16
TF ($SiC/ThCl_4$-$PuCl_3$)	BOC EOC	−5.301 −0.659	14,489
20TP40 ($SiC/ThCl_4$-$PuCl_3$)	BOC EOC	−1.886 −1.941	14,466
60TP40 ($SiC/ThCl_4$-$PuCl_3$)	BOC EOC	−1.836 −1.321	14,462
60TP40 ($YH_{1.85}/ThCl_4$-$PuCl_3$)	BOC EOC	−0.845 −0.089	10,730

4. Conclusions

The neutronic performance of a NaCl-$ThCl_4$-$PuCl_3$ fuel for Dual-Fluid Reactor was investigated using the Serpent Monte Carlo code. The results showed that decreasing the ^{239}Pu content reduced the fuel cycle length, and the $YH_{1.85}$ moderator improved thorium utilization and extended the fuel cycle length in the reference geometry. The replacement of $^{238}UCl_3$ with $ThCl_4$-$PuCl_3$ blanket significantly increased the breeding performance, thus resulted in extended fuel cycle length about 14,460–14,490 EFPD, nearly 40 years of full-power operation. In this configuration, the cycle length was almost independent of the plutonium composition. The fuel temperature coefficients were negative for all investigated cases. However, they became small at the end of cycle for the thorium-based blanket cases (down to −0.089 pcm/K), thus, statistical uncertainties should be considered.

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