A Chloride and Fluoride Hybrid Salt Fuel for Passively-cooled Molten Salt Fast Reactor

Luqman Hasan Nahari^a, Yonghee Kim^{a*},

^aNuclear and Quantum Engineering, Korea Advanced Institute of Science and Technology (KAIST), 291 Daehak-ro, Yuseong-gu, Daejeon 34141, Republic of Korea *Corresponding author: yongheekim@kaist.ac.kr

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1. Introduction

Among the six Generation IV reactor types, the molten salt reactor is a nuclear reactor that utilizes liquid fuels, typically molten fluoride or chloride salt. Molten salt reactors (MSRs) offer some merits compared to the other Gen IV reactors. Regarding safety, the MSRs offer lowpressure operation, no danger of fuel melting, continuous online refuelling, easy removal of noble gases, and a selfregulating core that can follow demand loads with minimal use of control rods or none at all. Regarding economics, the MSRs have a compact structure, no need for fuel fabrication, and no need to shut down for refuelling. Regarding environmental aspects, the MSR can utilize thorium and recycle actinide, which decreases waste production from other light water reactors (LWRs) and reduces waste heat [1].

The i-SAFE-MSR research center has been established to develop an innovative natural circulation molten salt fast reactor design named PMFR (the Passively-Cooled Molten Salt Fast Reactor). The key concepts and requirements of the PMFR consist of [2]:

- Operation of natural circulation on the primary system
- Separation of non-soluble fission products
- Severe-accident-free and passive safety system
- Long-lifetime core design
- Corrosion-resistant base material and coating in molten salts

 Original multi-physics numerical analysis platform Many works have been done to develop long-lived and high-burnup MSFRs. This paper introduces a preliminary fuel salt study for chloride and fluoride hybrid salt fuel compared with binary and ternary salt regarding neutronic parameters such as burnup, conversion ratio, energy spectrum, and temperature coefficient. These three papers [3], and [4] provide more details regarding the material and design specifications.

2. Methods and Results

2.1 Design Configuration

The PMFR design implements an integral single-fluidtype MSR configuration. The fuel salt and secondary heat exchanger location is inside the reactor vessel. The detailed schematic configuration of the PMFR is illustrated in Figure 1, while the specification design can be found in Table 1.



Figure 1 shows the reactor design, consisting of a cylindrical core with a 100 cm diameter and a height of 195 cm of active core. A moderator surrounds the core, and the reflector with each component has a 40 cm thickness. The inner surface of the core is coated with Hastelloy-N, which is 0.1 cm thick to prevent corrosion.

Table 1. Orandin-based motion sait cutectic data [5][6]					
Candidate Fuel salt	KCl-UCl ₃	NaCl-KCl- UCl ₃	KCl-UCl ₃ - UF ₄		
Molar composition [%]	46-54	42.9-20.3- 36.8	28.0-36.0- 36.0		
Eutectic temperature (°C)	558	470.15	475		
Uranium density (g/cm ³)	2.07	1.702	2.99		
Heat Capacity [J·kg ⁻¹ K ⁻¹]	465.76	567.78	440.45		

Table I: Uranium-based molten salt eutectic data [5][6]

Two primary requirements for selecting fuel salt are sufficiently high heavy metal composition and low melting temperature. Table 1 shows fuel salt candidate properties that fulfill this requirement. For all fuel salt candidates, the Cl-37 is enriched as 99 at.%. A higher total fissile mass also results in a higher fuel composition. Among the salts, KCl-UCl₃-UF₄ has the most enormous mass of uranium, and NaCl-KCl-UCl₃ has the smallest. This research selects chloride and fluoride hybrid fuel salts (KCl-UCl₃-UF₄).

The control drums were positioned within the moderator region and covered with a pad with a buffer region between the layered components. The design involves 8 drums with a 120° angle of pads encircling the PMFR active core with a 24.74 cm radius of the drums. Beryllium Oxide (BeO) is used for the moderator material with 3.01 g/cm³. In addition, shutdown plate devices are adopted to handle a high excess reactivity at cold zero power (CZP). The control drum specification and shutdown plate specification are defined in Table II and Table III, while its configuration details are shown in Figures 1 and 2, respectively.

Control Drum Parts	Material	Thickness [cm]
Pad	B ₄ C (95% B-10 enrichment)	5.3
Layer	SS-304	0.03
Buffer	Helium Gas at 823 K	0.2
Guide Tube	SS-304	0.03

Table III: Shutdown plate specification

Shutdown Plate Parts	Material	Thickness [cm]
Pad	B ₄ C (95% B-10 enrichment)	2 cm
Hollow space	Helium	2 cm



Figure 2. Shutdown Plate Configuration

Maintaining reactivity below 1000 pcm is vital to ensure the implementation of the Burnable Absorber (BA). Two shape models of BA are adopted in this reactor: rod type and pad type. The BA is coated with a 0.5 mm thickness of SS-304. Table IV demonstrates the BA configuration summary in this model, illustrated in Figure 3.

Table IV: BA configuration summary of the previous and optimized model

optimized model					
ВА Туре	Radius Size [mm]/ angle [°]	Total Qty	No. of Layer		
	9.75	8	6		
	9.5	8	5		
Rods	8.0	8	4		
	6.0	16	2		
	5.3	16	1		
Pads	20.2	1	2.75 mm thickness - 0 mm distance		
	12.2	1	2.0 mm thickness - 0 mm distance		
	16	1	1.5 mm thickness - 0 mm distance		
	24	1	0.85 mm thickness - 0 mm distance		
	60	1	0.75 mm thickness - 0 mm distance		



Figure 3. BA Configuration

2.2 Numerical Results

The calculations were conducted using the Monte Carlo Serpent 2 code, version 2.2.1, with the ENDF/B-VII.1 nuclear library. For the depletion calculation, 10,000,000 histories were simulated, which involved 50,000 particles and 300 cycles, with the first 100 cycles ignored from the results. The burnup step was performed annually for a 300 MWth power output with 923 K without considering fuel salt movement effects. More detailed comparisons are discussed in the following section.



Figures 4 and 5 illustrate the neutronic performance of PMFR. Using 19.75 % enrichment, the reactor lifetime reaches almost 100 years. However, it is impossible to implement the BA surrounding the core due to high initial excess reactivity. The enrichment is decreased from 19.75% to 15% to maintain excess reactivity below 1000 pcm using BA. Then, the reactor's lifetime is 58 years. Figure 6 shows that the burnup at the end of life (EOL) is 72.93 MWd/kgU with a conversion ratio of 0.672.



Figure 5. Detailed depletion result for KCl-UCl₃-UF₄ (15% enrichment) w/ BA



Figure 6. Burnup and conversion Ratio for KCl-UCl₃-UF₄ (15% enrichment) w/ BA



Figure 7. Energy spectrum for KCl-UCl_3-UF4 (15% enrichment) w/ BeO moderator w/ BA

Figure 7 shows the energy spectrum of the active core of the reactor at the beginning of life (BOL) and end of life (EOL). Due to BeO being implemented as a moderator outside the core, some neutrons are in the thermal region. In addition, at EOL, the energy spectrum becomes softer due to decreased fissile fuel content and accumulation of fission products.

The temperature coefficient is calculated by varying the material temperature from 823 K to 1023 K according to the molten salt's inlet temperature of 873 K and outlet temperature of 923 K. The temperature coefficient includes the fuel temperature coefficient (FTC), reflector temperature coefficient (RTC), and isothermal temperature coefficient (ITC). These parameters are calculated at BOL with and without BA.

Table IV: Temperature co	efficient evaluation	1 for	· KCl-UCl ₃ -
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UF ₄ (19.75% Enrichment) w/ BeO Moderator w/o BA				
Temperature Range (K)	823-923	923-1023	823-1023	
FTC (pcm/K)	-2.44±0.05	-2.55±0.08	-2.50 ± 0.03	
RTC (pcm/K)	0.78±0.05	0.65±0.05	0.72±0.03	
ITC (pcm/K)	-1.68±0.05	-1.81±0.05	-1.75±0.03	

Table V: Temperature coefficient evaluation for KCl-UCl₃-UF4 (15% Enrichment) w/ BeO Moderator w/o BA

Temperature	823-923	923-1023	823-1023
Range (K)			
FTC (pcm/K)	-2.53±0.07	-2.65±0.07	-2.59 ± 0.04
RTC (pcm/K)	1.12±0.07	1.04 ± 0.07	1.08 ± 0.04
ITC (pcm/K)	-1.59±0.07	-1.55±0.07	-1.58 ± 0.04

Table VI: Temperature coefficient evaluation for KCl-UCl₃-

UF4 (15% Enrichment) W/ BeO Moderator W/ BA					
Temperature	823-923	923-1023	823-1023		
Range (K)					
FTC (pcm/K)	-7.09±0.08	-7.61±0.08	-7.35±0.04		
RTC (pcm/K)	0.47 ± 0.08	0.05 ± 0.08	0.26 ± 0.04		
ITC (pcm/K)	-6.84±0.08	-7.48±0.08	-7.16±0.28		

Tables IV and V demonstrate that, using lower enrichment, the FTC has become slightly more negative compared to the 19.75% enrichment case. Meanwhile, the RTC is slightly more positive than the 19.75% enrichment case. Both phenomena occur because the U-238 is higher, which means the Doppler broadening of U-238 is stronger. As a result, decreasing uranium enrichment generally makes the FTC more negative.

Tables V and VI demonstrate that the FTC at BOL for KCl-UCl₃-UF₄ with BA is higher, with a value of -7.09 pcm/K at 823-1023 K compared to without BA. On the other hand, the RTC is quite similar, with a slightly positive value because the nuclei in the moderator experience a hardening spectrum, which decreases the probability of parasitic capture. The ITC indicates the change in reactivity per degree of temperature change in both fuel and moderator/reflector. The ITC without a BA at a range of 823-1023 K is -1.75 pcm/K, and with BA is -7.35 pcm/K, indicating inherent safety. Nevertheless, using BA to maintain excess reactivity below 1000 pcm has a drawback: it is quite challenging at low temperatures, such as cold zero power (CZP), due to high excess reactivity.

Table VI: Control drum worth summary at BOL at operational temperatures 923 K (15% Enrichment)

Case		k _{eff}	Reactivity [pcm]		Control Drum Worth [pcm]	
		Value	Value Unc.		Value	Unc
DOI	Drum Out	1.01001	991	15	2,000	22
BOL	Drum In	0.98330	-1698	16	2089	22
MOI	Drum Out	1.00458	456	14	4540	21
MOL	Drum In	0.96068	-4093	15	4349	21
EOL	Drum Out	1.00112	112	14	7404	21
	Drum In	0.82367	-7372	16	7464	21

Table VI summarizes the control drum worth in 3 varied operation times. At the beginning of life (BOL) at drum-in condition, the reactor undergoes a subcritical at 0.98330 with a control drum worth 2678 pcm, which is quite small. Since the reactor has high excess reactivity due to higher fuel content, further investigation is required to increase the control drum's worth, such as decreasing the enrichment, which makes the reactor's lifetime shorter.

The shutdown margin is the amount of negative reactivity needed for the reactor to be in a subcritical state when all reactivity control mechanisms, except the most reactive one, are fully inserted into the core. The calculation utilized 300,000 particles with 100 inactive and 200 active cycles to reach uncertainty below 10 pcm. The theoretical density of KCl-UCl₃-UF₄ is 5.3027 g/cm³ at 298 K and 4.5765 g/cm³ at 873 K according to inlet temperature. Table VII shows the control drum's worth and shutdown margin at BOL under hot zero power (HZP) temperature conditions. However, the implementation of shutdown safety devices (shutdown plate) is not guaranteed to get enough shutdown margin at CZP.

Table VII: SDM evaluation (15% Enrichment) at HZP with a temperature of 873 K

Case	k _{eff}	Drum Worth [pcm]	Single Drum Worth [pcm]	SDM [pcm]
All DO*	1.01740	2500		
All DI*	0.99217	2300	-	-
D1 Out	0.99417	2310	190	583

*DO =Drum Out, DI = Drum In

Table VIII: SDM evaluation ((15% Enrichment)) at CZP with a temperature of 298 K

Case	k _{eff}	Drum Worth [pcm]	Single Drum Worth [pcm]	SDM [pcm]
All DO	1.05391	1669		
All DI	1.03570	1668	-	-
D1 Out	1.03715	1758	-	-



Figures 8 and 9 are radial flux distributions of total neutron and thermal neutron at BOL and EOL conditions,

respectively. Thermal neutron only shows up in the moderator and reflector areas.



3. Conclusions

The neutronic calculations for fluoride and chloride hybrid fuel salt have been done. The reactor's lifetime is 58 years with 72.93 MWd/kgU. The installation of a control drum can increase the reactor safety system with its drum worth from 2680 to 7484 throughout the operation. At CZP, the shutdown margin is not guaranteed because the initial excess reactivity is too high. Further evaluation is required to ensure the shutdown margin at CZP and HZP.

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