Fuel Comparison Study for a Passively-cooled Molten Salt Fast Reactor between NaCl-KCl-UCl_3 and KCl-UCl_3

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1. Introduction

The Molten Salt Reactor is one of the Generation IV nuclear reactor designs that can use actinides to produce electricity, hydrogen, and fissile fuels using liquid fuels, typically molten fluoride or chloride salt, as fuel and coolant. Molten Salt Reactors (MSRs) have several advantages such as including low-pressure operation and continuous online refueling, economic benefits such as compact structure and high-temperature operation without the need for shutdowns, and environmental advantages such as Thorium utilization, Actinide recycling to reduce waste production, and decreased waste heat generation compared to Light Water Reactors (LWRs) [1].

The i-SAFE-MSR research center in the Republic of Korea has been established To develop an innovative natural circulation molten salt fast reactor design called PMFR (the Passively-Cooled Molten Salt Fast Reactor). The fundamental concepts and requirements of the PMFR are outlined below [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

In prior studies, several analyses have been conducted, including burnup, conversion ratio, control drum worth, and power distribution. More comprehensive details on materials and design are available in these three papers [3], [4], and [5]. Nevertheless, in the prior studies [5], the shutdown margin is not sufficient at Cold Zero Power (CZP) at the Beginning of Life (BOL). Introducing new fuel salt using ternary salt (NaCl-KCl-UCl3) can be considered to tackle this issue. This research compares NaCl-KCl-UCl_3 and KCl-UCl_3 fuel salts regarding neutronic parameters such as control drum worth, conversion ratio, energy spectrum, and shutdown margin.

2. Methods and Results

The calculations were performed using the Monte Carlo Serpent 2 code, version 2.2.1, with the ENDF/B-VII.1 nuclear library. For the burnup scheme, simulations use 30,000,000 histories involving 100,000 particles and 500 cycles, with the first 200 cycles excluded from the results. The depletion step was conducted annually over 40 years for a 300 MWth power output. The reactor simulation was carried out at 923 K, and the study did not account for any fuel salt movement effects. Both designs should keep their reactivity swing below 1,000 pcm, utilizing a 40 cm BeO moderator with a burnable absorber (BA) and a control drum installed [5]. More detailed comparisons are discussed in the following section.

2.1 Design Configurations

Table I: Design Configuration Differences

Parts	Specifications	Case	
		KCl-UCl_3	NaCl-KCl-UCl_3
Fuel	Molar Composition	46-54	42.9-20.3-36.8
	Melting Temperature (°C)	558	470
	Density (g/cm^3) at 923 K	3.789	3.364
Burnable Absorber	B-10 Enrichment (%)	95	19.9 (Natural)
Control Drum	Total Unit	20	16
	Radius (cm)	17.95	23.74

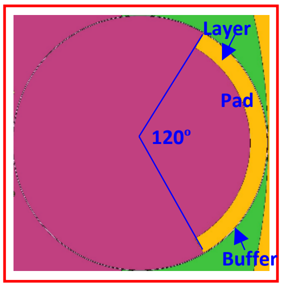

Fig. 1. KCl-UCl_3 model (left) and NaCl-KCl-UCl_3 model (right) control drum parts

Table I mentions that both molar compositions for fuel salt are based on eutectic points. B_4C density for the KCl-UCl_3 model is higher due to accommodating higher initial reactivity. Meanwhile, the B_4C density for the NaCl-KCl-UCl_3 model is lower due to lower initial reactivity and to accommodate helium gas thermal expansion produced from boron-neutron capture (^{10}B(n, α)^{7}Li). In addition, the total control drum for the NaCl-KCl-UCl_3 case is much lower than the other one because the initial reactivity is much less than the KCl-UCl_3 model. However, to maximize the shutdown margin in the NaCl-KCl-UCl_3 model, the control radius is much bigger than the other one. Both designs feature control drums positioned within the moderator region, consisting of a B_4C pad (B-10 enrichment at 95%) with a buffer zone between the layered components. Detailed KCl-UCl_3 and NaCl-KCl-UCl_3 control drum configurations are illustrated in Figures 2 and 3.

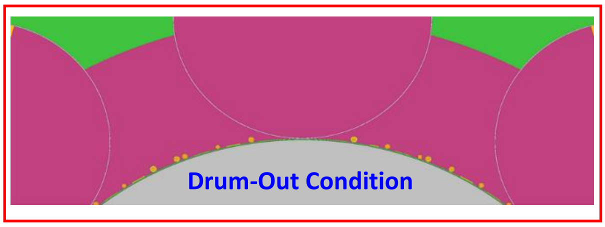

Fig. 2. Configuration of KCl-UCl_3 case, all drum-out conditions in X-Y plane

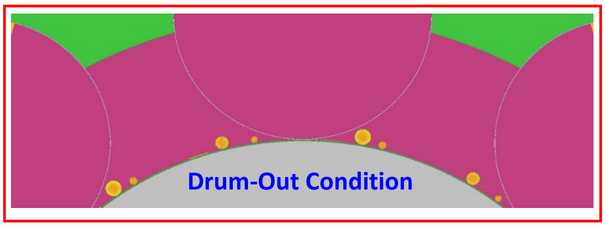

Fig. 3. Configuration of NaCl-KCl-UCl3 case, all drum-out conditions in X-Y plane

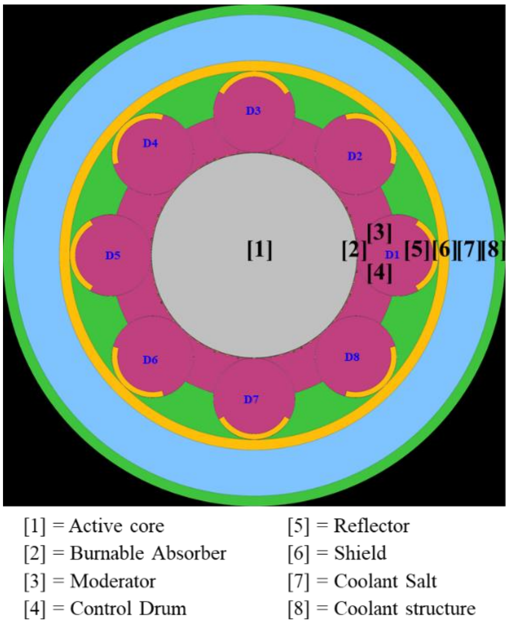

Fig. 4. Control drum-in conditions (KCl-UCl_3 Model)

Due to the different fuel content in both designs, The KCl-UCl3 model implements 20 control drums with a radius of 17.95 cm; meanwhile, the NaCl-KCl-UCl_3 adopts 16 control drums with a radius of 23.74 cm. This difference in configurations requires different BA configurations for each model to keep the reactivity swing below 1,000 pcm. Two types of BAs are used in reactors: rod type and pad type, both coated with a 0.5 mm layer of SS-304. Table II summarizes the BA configurations in the KCl-UCl_3 and NaCl-KCl-UCl_3. The NaCl-KCl-UCl_3 models are illustrated in Figure 4.

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

Case	KCl-UCl_3 Model			NaCl-KCl-UCl_3 Model		
BA Type	Radius Size [mm]/ angle [°]	Total Qty	No. of Layer/ Thickness [mm]	Radius Size [mm]/ angle [°]	Total Qty	No. of Layer/ Thickness [mm]
Rods	10.5	8	6	25	8	6
	9.5	8	5	20.5	8	5
	9.0	8	4	12.0	8	4
	8.4	16	2	10.5	8	2
	6.7	16	1			
Pads	40.2	1	2/2.5	3.5	14	2/2.5
	48	1	2/1.25			
	48	1	1/0.65			
	16	1	1/0.2	3.5	2	2/2
	8	1	1/0.1			

2.2 Burnup Calculation

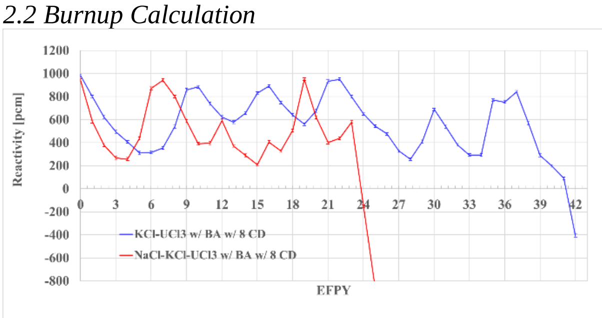

Fig. 5. Reactivity profile comparison

Based on Table III, introducing NaCl-KCl-UCl3 fuel salt in the BA and Control Drum configuration decreases the PMFR's lifetime by 17.78 years compared to the KCl-UCl_3 model, as shown in Figure 5. Also, the reactivity fluctuations appear because Burnable absorbers of different sizes deplete at different rates, providing a more finely tuned compensation for the reactivity loss. Different sizes of burnable absorbers deplete at different rates, allowing for more precise control over time. Smaller or less concentrated absorbers will deplete faster, providing short-term control, while larger or more concentrated ones provide longer-term reactivity suppression. Additionally, the reactivity profile in both models is successfully maintained between 0 and 1,000 pcm throughout the reactor's lifetime.

Table III: Burnup and conversion ratio at EOL

Case	Burnup at EOL [MWd/kgU]	Conversion Ratio	Lifetime
KCl-UCl_3	113.67	0.477	41.07
NaCl-KCl-UCl_3	80.46	0.437	23.79

2.3 Energy Spectrum

Figure 6 compares the energy spectrum of the PMFR between the KCl-UCl_3 and NaCl-KCl-UCl_3 models. The

$NaCl-KCl-UCl_3$ model has a softer spectrum due to the high fraction of NaCl and KCl, contributing to moderating neutrons from the Beginning of Life (BOL) until the End of Life (EOL).

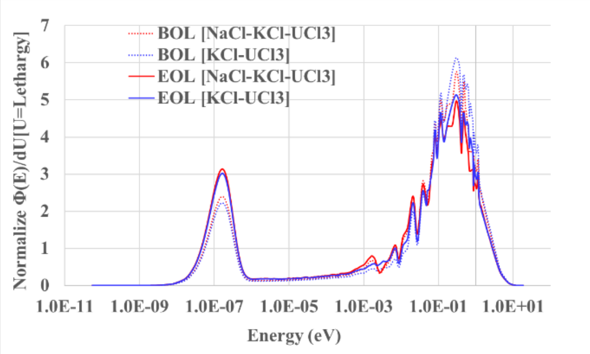

Fig. 6. The energy spectrum of PMFR

2.4 Temperature Coefficient

The temperature coefficient calculation was performed by varying the material temperature from 823 K to 1023 K based on the molten salt's inlet temperature of 600 °C and outlet temperature of 700 °C. The temperature coefficient includes the Fuel Temperature Coefficient (FTC), Reflector Temperature Coefficient (RTC), and Isothermal Coefficient (ITC). These parameters were observed at the Beginning of Life (BOL) conditions. "Unc." stands for uncertainty.

Table IV: Temperature coefficient evaluation at BOL

Parameter	Case	Temperature Coefficient [pcm/K]	
		Value	Unc.
FTC	$KCl-UCl_3$	-13.57	0.03
	$NaCl-KCl-UCl_3$	-10.72	0.03
RTC	$KCl-UCl_3$	0.25	0.03
	$NaCl-KCl-UCl_3$	0.65	0.03
ITC	$KCl-UCl_3$	-13.32	0.06
	$NaCl-KCl-UCl_3$	-10.07	0.06

Table IV shows that the FTC at BOL for the $KCl-UCl_3$ model is higher with a value of -13.57 pcm/K than the other one because the total number of BA is much higher in this case. On the other hand, the RTC for the $KCl-UCl_3$ has a positive value of 0.25 pcm/K but is much lower than the other one due to a higher number of BA. The nuclei in the moderator experience a hardening spectrum due to the temperature increase, which reduces the likelihood of parasitic capture. If the moderator has sufficient thickness, it can enhance neutron absorption in the fuel, resulting in a slightly positive RTC value. The ITC represents the change in reactivity per degree of temperature change in both the fuel and moderator/reflector. The ITC is calculated simply by summing the RTC and FTC, yielding a value of -13.32 pcm/K for the $KCl-UCl_3$ model and -10.07 pcm/K for the $NaCl-KCl-UCl_3$ model at BOL. Both of them have negative temperature reactivity coefficients, indicating inherent passive safety. However, controlling the reactor at low temperatures can be challenging due to excess reactivity. Therefore, optimizing the drum control is essential to ensure a sufficient shutdown margin or rod worth at low temperatures.

2.5 Control Drum Worth

The control drum worth was determined by calculating the difference in reactivity between the drum-out and drum-in conditions at the Beginning of Life (BOL). The all-drums-in configuration for the $KCl-UCl_3$ model is illustrated in Figure 4. Tables V and VI summarise the control drum worth at BOL under operational temperatures (923 K) for both cases.

Table V: Control drum worth summary at BOL at operational temperatures 923 K ($KCl-UCl_3$ model)

Case		k_{eff}	Reactivity [pcm]		Control Drum Worth [pcm]	
		Value	Value	Unc.	Value	Unc.
BOL	Drum Out	1.00982	972	13	6165	19
	Drum In	0.95064	-5193	16		
MOL	Drum Out	1.00681	676	13	11003	18
	Drum In	0.90640	-10327	15		
EOL	Drum Out	1.00091	91	13	18619	18
	Drum In	0.84368	-18528	14		

Table VI: Control drum worth summary at BOL at operational temperatures 923 K ($NaCl-KCl-UCl_3$ model)

Case		k_{eff}	Reactivity [pcm]		Control Drum Worth [pcm]	
		Value	Value	Unc.	Value	Unc.
BOL	Drum Out	1.00952	943	13	10142	20
	Drum In	0.91576	-9199	15		
MOL	Drum Out	1.00398	396	12	14882	19
	Drum In	0.87347	-14486	15		
EOL	Drum Out	1.00583	580	12	21988	19
	Drum In	0.82367	-21408	15		

At BOL for the $KCl-UCl_3$ model, when the control drums are in the drum-in position, the PMFR achieves a subcritical phase with a k_{eff} of 0.95064. Meanwhile, the $NaCl-KCl-UCl_3$ model achieved a k_{eff} of 0.91576. Although the number and the geometry size of the control drum are the same, some differences exist in the control drum worth. This difference appears because, in the $NaCl-KCl-UCl_3$ model, the fuel content is also more minor compared to $KCl-UCl_3$. Tables V and VI show that both control drum's worth models can be assumed to meet the shutdown margin requirements at BOL at the Hot Full Power (HFP) temperature of 923 K.

2.6. Shutdown Margin

The Shutdown Margin (SDM) is the amount of negative reactivity required for the reactor to reach a subcritical state when all reactivity control mechanisms, except the most reactive control drum, are fully inserted into the core. This calculation used 1,000,000 particles with 200 inactive and 300 active cycles, ensuring an uncertainty value below 10 pcm. Table VII evaluates the control drum worth and shutdown margin at BOL under Hot Zero Power (HZP) temperature conditions.

The theoretical density of KCl-UCl_3 at 298 K is 4.56035 g/cm³. Meanwhile, for Hot Zero Power (HZP) calculations, the fuel salt density is 3.85093 g/cm³ at 873 K, corresponding to the inlet temperature. Tables VII and VIII provide the shutdown margin evaluation at BOL under HZP and CZP conditions.

On the other hand, At 298 K, the theoretical density of NaCl-KCl-UCl_3 is 4.00227 g/cm³. For Hot Zero Power (HZP) calculations, this density adjusts to 3.41577 g/cm³ at 873 K. Tables IX and X present the shutdown margin evaluations at BOL under HZP and Cold Zero Power (CZP) conditions.

Table VII: SDM evaluation (KCl-UCl_3 configuration) at HZP with a temperature of 873 K

Case	k_{eff}	Drum Worth [pcm]	Single Drum Worth [pcm]	SDM [pcm]
All DO	1.016540	5954	-	-
All DI	0.958530			
D1 Out	0.965395	5212	742	3461

Table VIII: SDM evaluation (KCl-UCl_3 configuration) at CZP with a temperature of 298 K

Case	k_{eff}	Drum Worth [pcm]	Single Drum Worth [pcm]	SDM [pcm]
All DO	1.086240	3867	-	-
All DI	1.042450			
D1 Out	1.047390	3415	452	-

Under Hot Zero Power (HZP) conditions, with all control drums in the drum-in position, the KCl-UCl_3 model is in a subcritical phase with a k_{eff} of approximately 0.958 and a total drum worth of 5954 pcm. The shutdown margin achieved 3461 pcm, which indicates that all control drums can compensate for the excess reactivity when transitioning from Hot Full Power (HFP) to HZP conditions. Meanwhile, at CZP, the shutdown margin is not sufficient due to high reactivity at BOL. As a note, the control drum and BA configuration are almost symmetrical in the xy direction, so the control drum worth and shutdown margin are likely similar.

Table IX: SDM evaluation (NaCl-KCl-UCl_3 configuration) at HZP with a temperature of 873 K

Case	k_{eff}	Drum Worth [pcm]	Single Drum Worth [pcm]	SDM [pcm]
All DO	1.014540	9824	-	-
All DI	0.922587			
D1 Out	0.935792	8295	1530	6421

Meanwhile, at Hot Zero Power (HZP), with all control drums in the drum-in position, the NaCl-KCl-UCl_3 model is in a subcritical phase with a k_{eff} of approximately 0.922 and a total drum worth of 9824 pcm. Similarly, at Cold Zero Power (CZP), the shutdown margin is insufficient to compensate for the excess reactivity in CZP.

Table X: SDM evaluation (NaCl-KCl-UCl_3 configuration) at CZP with a temperature of 298 K

Case	k_{eff}	Drum Worth [pcm]	Single Drum Worth [pcm]	SDM [pcm]
All DO	1.067660	6581	-	-
All DI	0.997565			
D1 Out	1.007430	5600	982	-

3. Conclusions

Neutronic calculations for both models have been conducted. The reactor's lifetime for the KCl-UCl_3 model is 41.07 years, almost 2 times longer than that of the other model. Although both models have the shutdown margin at CZP is not sufficient due to high initial excess reactivity, the NaCl-KCl-UCl_3 fuel salt model is preferable due to its material capability, which stands for over 20 years and is much easier to fabricate than over 40 years. Further investigation is needed to maximize burnup and enhance the utilization of fuel.

REFERENCES

[1] T. J. Dolan, "1 - Introduction," in *Molten Salt Reactors and Thorium Energy*, T. J. Dolan, Ed., Woodhead Publishing, 2017, pp. 1–12. doi: https://doi.org/10.1016/B978-0-08-101126-3.00001-4.

[2] J. PARK et al., "Design Concepts and Requirements of Passive Molten Salt Fast Reactor (PMFR)," in *Transactions of the Korean Nuclear Society Spring Meeting*, South Korea, 2022.

[3] N. N. Aufanni, E. Lee, T. Oh, and Y. Kim, "[ICAPP 2023] Burnable Absorber Design Study for a Passively-Cooled Molten Salt Fast Reactor," *Nuclear Engineering and Technology*, 2023, doi: 10.1016/j.net.2023.11.001.

[4] N. N. Aufanni, E. Lee, and Y. Kim, "Control Drum Design Optimization for a Passively-Cooled Molten Salt Fast Reactor." in Reactor Physics Asia 2023 (RPHA2023) Conference, South Korea, 2023.

[5] L. H. Nahari, N. N. Aufanni, E. Lee, and Y. Kim, "Shutdown Margin Study for a Passively-cooled Molten Salt Fast Reactor," in *Transactions of the Korean Nuclear Society Spring Meeting*, South Korea, 2024.