

# Study on Some Neutronics Behavior of Low Enriched Uranium Salt Composition Proposed for a Molten Salt Reactor (MSR) Using the OpenMC Monte Carlo Method

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**Abstract:** The molten salt reactor (MSR) is a type of GEN-IV advanced reactor that uses melt combinations of heavy metal elements and molten salt as fuel and coolant. Molten salt reactors (MSRs) are fourth-generation reactors that are built to be safe, have no risk of core meltdown, and can be fed and processed online. This study examines the neutronics properties of a conventional MSR using Monte-Carlo and OpenMC codes. MSR cores with varying low-enriched  $^{235}\text{U}$  coolant salt compositions were tested to determine the optimal fuel salt composition. To assess non-proliferation, neutronics and safety were tested on low-enriched uranium fuel with different coolant salt compositions for MSR. OpenMC was used to create and simulate eight reactor cores with various fuel compositions. These computations were completed in 35 cycles, with 3000 particles per cycle, while 5 cycles were skipped to avoid statistical errors. For fission rates, temperature reactivity feedback, conversion ratio, and neutron spectra calculations, statistical errors were reduced to 1.9% and 63 pcm for keff values, respectively. All computations are performed using the nuclear data libraries JEFF3.3 and END/B VIII.0. The burnup of fissionable materials and neutron toxicity were investigated. The fission rates of U-235, Pu-239, Xe-135 and Pu-241 were investigated in relation to burnup. The neutronic evaluation of standard fuel salt composition for the ORNL molten salt reactor was performed using OpenMC during normal operation and compared to the experimental value in terms of effective multiplication factor for validation (keff), which was 0.06%. MSRs are passively safe because of the negative temperature reactivity coefficient of fuel salt. Because of their increased atom density, conversion ratio, and FoM, cooling salts like 73%LiF-27%UF<sub>4</sub> may be suitable carrier salts. This study outlines the problems, challenges, and development trends for MSR multi-physics models in order to guide future research. This work serves as a reference for molten salt reactor core design using an ideal fuel salt composition of 73% LiF-27%UF<sub>4</sub>.

**Key words:** low enriched, uranium salts, reactor, molten, OpenMC, multiplication factor, burnup

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## 1. Introduction

Molten salt reactor (MSR) is an advanced next generation nuclear reactor type. The concept of MSR was first proposed in the 1950s and 1960s and was explored in the Molten Salt Reactor Experiment (MSRE) at Oak Ridge National Laboratory in the 1960s [1] [2]. In recent years, there has been renewed interest in MSRs due to their potential for improved safety, efficiency, and reduced waste compared to traditional nuclear reactors. One of the main advantages of molten salt reactors (MSRs) is their use of liquid fuel, which allows for higher fuel utilization and reduced waste compared to traditional solid fuel reactors. Until now,  $^7\text{LiF-BeF}_2$  with the combination of high enriched Uranium has been the most popular fuel salt combination used [3]. Tritium production, beryllium toxicity, and proliferation concerns from this highly enriched Uranium make this fuel salt composition difficult to regulate. Lithium enrichment and Beryllium costs make carrier salt expensive also [4] [5]. This paper quantitatively explores the usage of recently suggested 8 different types of salt composition as a way to lessen or eliminate this additional load. Beginning of this work the conventional molten salt reactor by ORNL is

modelled using OpenMC Monte Carlo code. Some neutronics data associated with these fuel salt compositions are calculated using this code in regard to the justification of the scopes of proposal of mentioned fuel salt compositions. Another way to make a progress in MSR technology is the development of advanced fuel salt purification and reprocessing technologies, since this work is only focused to justify some neutronics parameter of the proposed salt compositions. The proposed study focuses on the neutronic properties of LEU-based salt fuel composition, such as reactivity, neutron flux distribution, and safety margins, in the context of emerging MSR designs. Only a few computational investigations on LEU salt compositions have been conducted using Monte Carlo methods such as OpenMC. Insufficient high-fidelity neutronics data for MSR design. There have been no comparison studies conducted between traditional solid fuel reactors and projected LEU salt MSRs. This study was conducted in response to these deficiencies, demonstrating the study's distinctiveness and innovation.

This study focuses on the neutronic behavior of the proposed LEU fuel salt using OpenMC and does not include

thermal-hydraulic coupling. We acknowledge that full safety and fuel-cycle assessments require such coupling and have noted this limitation in the manuscript. Future work will integrate thermal-hydraulic analysis with the neutronics results.

Based on the aforementioned study gaps, the following research question has been established:

Can OpenMC accurately predict the complicated geometries and compositions of LEU-based MSRs?

## 2. Methods and Methods

### 2.1 ORNL MSRE Description

ORNL MSRE model had a unique geometry design and model compared to traditional solid fuel reactors. The reactor vessel was a cylindrical container made of graphite, which was chosen for its thermal stability and ability to withstand high temperatures. The size of the vessel was approximately 4 meters in diameter and 8 meters in height, with a wall thickness of 23 cm. Figure 1 shows a cutaway simplified drawing of the MSRE reactor vessel [6].

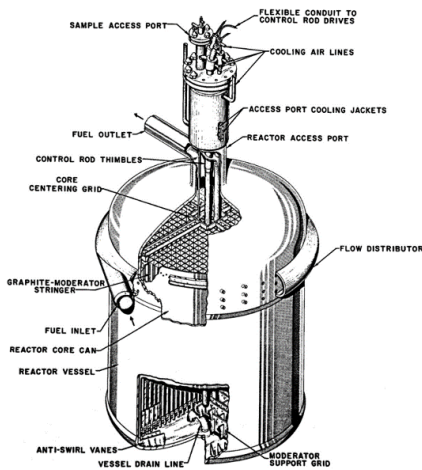


Fig. 1. Simplified cut way view reactor vessel of MSRE

The fuel system consisted of a liquid mixture of uranium and fluoride salts, which flowed through the core of the reactor vessel and the heat exchangers. The fuel was pumped through the system using an impeller, and the heat exchangers were placed at strategic points in the system to extract heat and convert it to electricity. The coolant system consisted of a secondary loop of water, which flowed through the heat exchangers and was used to generate steam for electricity production. The coolant system was designed to operate at low pressures and temperatures, reducing the risk of accidents and improving safety. Other geometry design parameters of the MSRE included the use of a beryllium reflector to increase neutron efficiency, the placement of control rods for regulating the nuclear reaction, and the incorporation of safety features such as a freeze valve and drain tank. Table 1 shows the main design parameter of ORNL MSRE model.

Table 1: Design parameter of ORNL MSRE model.

Fuel salt	LiF – BeF <sub>2</sub> – ZrF <sub>4</sub> – UF <sub>4</sub>
Coolant salt	LiF – BeF <sub>2</sub>
Moderator	Graphite
Salt containers	INOR-8
Cover gas	Helium

### 2.2 Model generation & Validation

A computer-aided design (CAD) model of the MSR, based on data adopted from Copenhagen atoms (regeneration ORNL MSRE model), was created for this research. CAD-based geometry in OpenMC using the DagMC toolbox was implemented; the control rods met the requirements of 70% Gd<sub>2</sub>O<sub>3</sub> and Al<sub>2</sub>O<sub>3</sub>. The model was validated through the use of the Monte Carlo approach with the OpenMC (version 0.13.2) software with the JEFF 3.3 and ENDF/B VIII library data sets. In the produced model, Neutron multiplication was found  $1.02195 \pm 523$  pcm which was validated with the benchmark data where neutron multiplication was  $1.02132 \pm 3$  pcm [7]. And the difference between the produced model & the benchmark data was 63 pcm. Fig. 2 and 3 show the cross-sectional views of modelled MSR and Fig. 4 shows the result of  $k_{eff}$  of the produced model by using OpenMC.

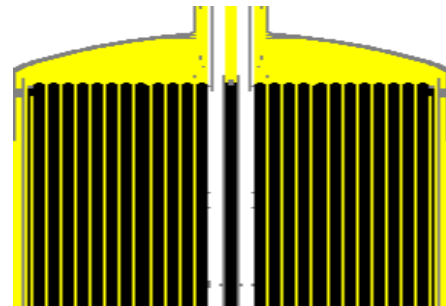


Fig. 2: Cross-sectional view of MSRE core (Vertical).

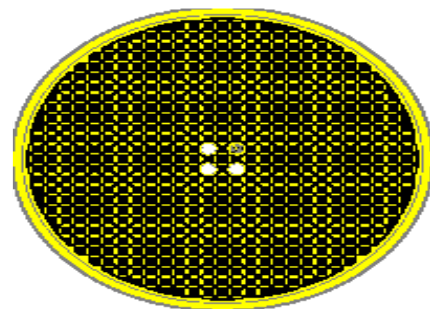


Fig. 3: Cross-sectional view of MSRE core (horizontal).

RESULTS	
k-effective (Collision)	= 1.02716 +/- 0.00596
k-effective (Track-length)	= 1.02835 +/- 0.00574
k-effective (Absorption)	= 1.01832 +/- 0.00496
Combined k-effective	= 1.02195 +/- 0.00523
Leakage Fraction	= 0.24453 +/- 0.00251

Fig. 4:  $k_{eff}$  of the produced model.

### 2.3 Convergence test for $k_{eff}$

Convergence study is performed to determine the optimal batch size for the simulation of MSR for getting a stable value of ( $k_{eff}$ ), taking into account the desired level of statistical uncertainty and computational efficiency. From the Fig. 5, it is seen that after taking 30 batch numbers the  $k_{eff}$  has become stable.

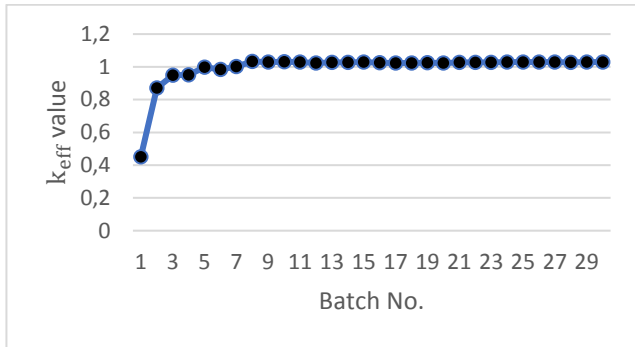


Fig. 5: Convergence of  $k_{eff}$  with the batch numbers.

### 2.4 Fuel salt choices

The financial repercussions of each salt option are thoroughly considered before final selection. For the sake of comparison, Table 2's first salt provides an estimate for FLiBe salt in which the Thorium fraction is substituted with Uranium. The highest Uranium content is found in the second salt, which is composed of 73%<sup>7</sup>LiF-27%UF<sub>4</sub>. As an added bonus, the absence of Beryllium in this salt makes it easier to develop new substances in the lab, as no special precautions related to Beryllium's toxicity are needed. Thirdly, 78%NaF-22%UF<sub>4</sub> has a higher melting point but no Lithium content, leading to Tritium production and poor economics. The melting point of the fourth salt (49% NaF-38%ZrF<sub>4</sub>-13%UF<sub>4</sub>) is lower than those of the previous three, but it still has the advantages of not containing Lithium and Beryllium [8]. Both the 58%NaF-30%BeF<sub>2</sub>-12%UF<sub>4</sub> and the 74%NaF-12%BeF<sub>2</sub>-14%UF<sub>4</sub> salts are made with the intention of lowering Zirconium parasitic absorption.

Table 2's seventh salt, 46%NaF-33%RbF-21%UF<sub>4</sub>, has many advantages, including a low melting point, a high Uranium capacity, and no Tritium production [8]. The final salt, 50.5%NaF-21.5%KF-28.2%UF<sub>4</sub>, has neither Beryllium nor Lithium in it. This results in a less dangerous salt, as there is no Beryllium to cause toxicity and no Lithium to cause Tritium production. Phase diagrams [9] [10] were used to estimate melting points of each salt, and the density of each salt was determined using the molar additions method [11] [12]. With the exception of 7 Li, which has been depleted to 99.995%, all of the salt's constituents are presented in their naturally occurring isotopic abundances. Table 2 lists the studied salt compositions.

Salt composition	Melting point[C]	Density [g/cm <sup>3</sup> ]
72%LiF-16%BeF <sub>2</sub> -12%UF <sub>4</sub>	480	3.353
73%LiF-27%UF <sub>4</sub>	490	4.340
78%NaF-22%UF <sub>4</sub>	618	4.056
49%NaF-38%ZrF <sub>4</sub> -12%UF <sub>4</sub>	540	3.757
58%NaF-30%BeF <sub>2</sub> -12%UF <sub>4</sub>	525	3.208
74%NaF-12%BeF <sub>2</sub> -14%UF <sub>4</sub>	500	3.437
46%NaF-33%RbF-21%UF <sub>4</sub>	470	4.026
50.5%NaF-21.5%KF-28%UF <sub>4</sub>	490	4.326

## 3. Results and Discussion

Main goal in the study is to determine optimum fuel composition from proposed fuel composition [5] through neutronic evaluation. The evaluated neutronics parameters were found out using tallies directly or indirectly.

### 2-D Fission Rate Distribution

The fission distribution provides the insights into the neutron transport, fission rates, and other important parameters that affect the reactor's performance. The horizontal view (Fig. 6) shows a heatmap, with bright lines indicating the number of fission events that occurred in each cell or region of the grid. The vertical view (Fig. 7) shows a cross-sectional view of the reactor, with contours representing the fission events at different depths within the reactor.

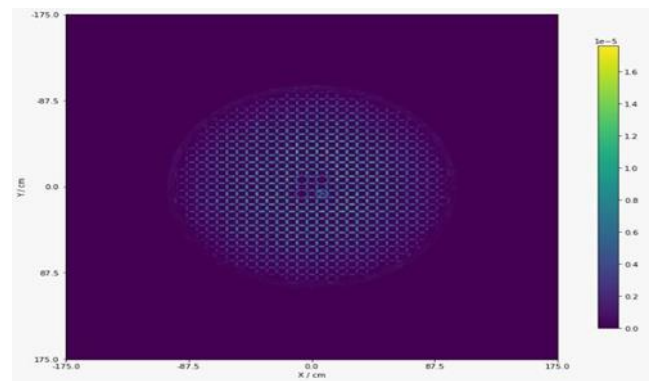


Fig. 6: 2-D fission rate distribution (horizontal).

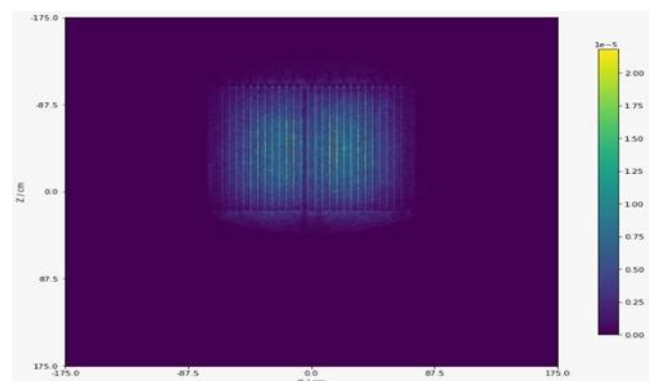


Table 2. Properties of the salts studied in the paper.

Fig. 7: 2-D fission rate distribution (vertical).

2-D Neutron Flux Distribution

2-D flux distribution of molten salt reactor is a visual representation of the spatial distribution of neutron flux in the reactor. The horizontal view typically shows a heatmap, with colours indicating the intensity of the neutron flux in each cell or region of the grid. The vertical view shows a cross-sectional view of the reactor, with contours representing the neutron flux at different depths within the reactor. The figures indicate that most of the flux is concentrated at the middle of the core. Fig. 8 and 9 shows the horizontal and vertical 2-D flux distribution.

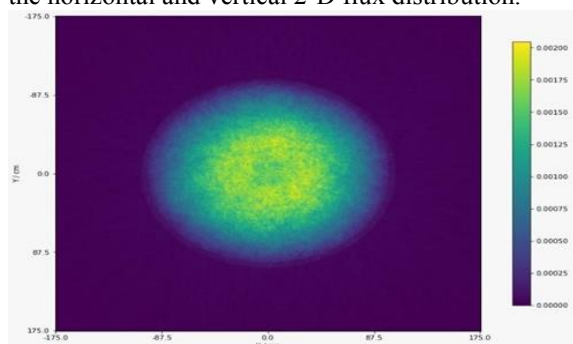


Fig. 8: 2-D neutron flux distribution (horizontal).

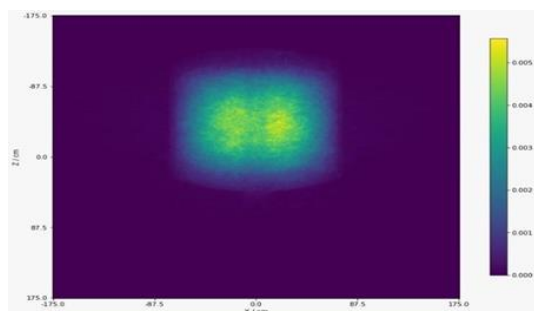


Fig. 9: 2-D neutron flux distribution (vertical).

Flux and Fission Distribution

Flux and fission distribution with respect to energy for a MSR is the representation of the energy distribution of neutrons in the reactor. Flux & fission both peak at thermal energy range (0.025eV). Because U-235 has maximum fission cross-section at thermal energy of about 585 barns, so the fission spectrum peaks at 0.025 eV. Almost all the neutrons are produced in the fast energy range through fission so flux increases at higher energies. Fig. 10 shows the fission (blue line) & flux distribution (Brown line) with respect to energy in logarithm scale.

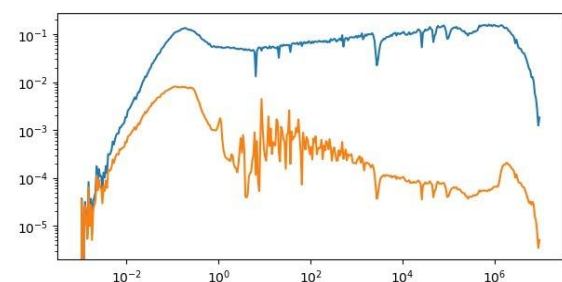


Fig. 10: Flux and fission distribution with respect to energy.

Critical Enrichment

$k_{eff}$  increases with the increase in enrichment of Uranium-235 as because the Uranium-235 enrichment level increases, the resonance absorption cross-section of Uranium-238 decreases due to the Doppler broadening effect. In MSR, the  $k_{eff}$  value tends to increase with an increase in the Uranium-235 enrichment level, as long as other factors remain constant (Figs. 11-18).  $k_{eff}$  increase with the increase of critical enrichment of the salt composition. Critical enrichment of the salt compositions ranges in between 7.5%-12% which result support the lower enrichment criteria. The results are enlisted in Table 3.

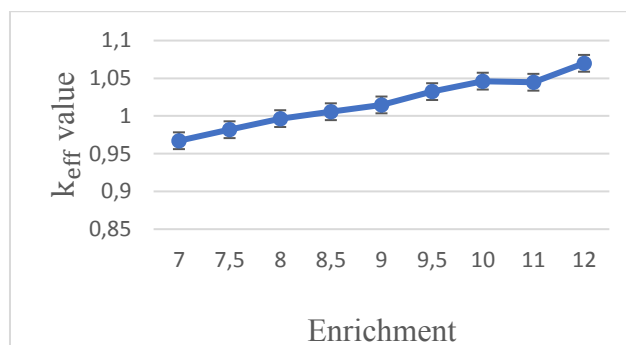


Fig. 11: Variation of  $k_{eff}$  with respect to enrichment for sample 1. (72%LiF-16%BeF<sub>2</sub>-12%UF<sub>4</sub>)

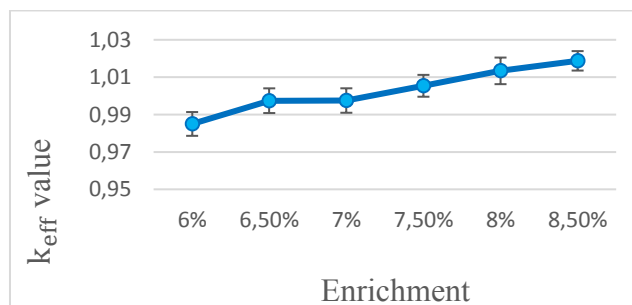


Fig. 12: Variation of  $k_{eff}$  with respect to enrichment for sample 2. (73%NaF-27%UF<sub>4</sub>)

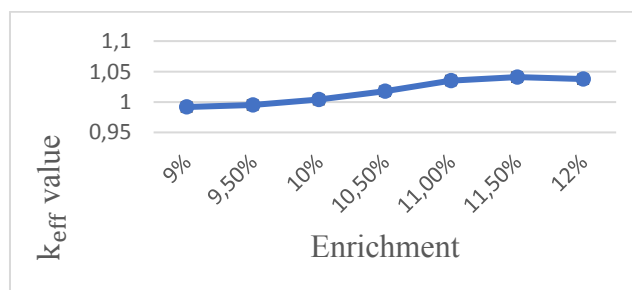


Fig. 13: Variation of  $k_{eff}$  with respect to enrichment for sample 3. (78%NaF-22%UF<sub>4</sub>)

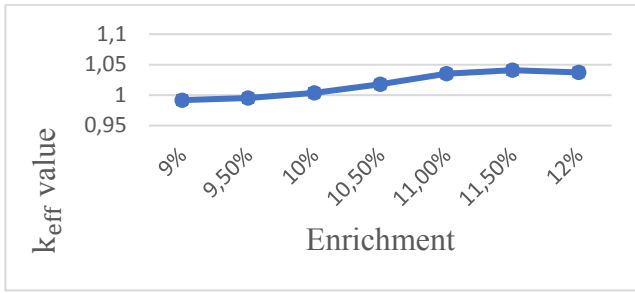


Fig. 14: Variation of  $k_{eff}$  with respect to enrichment for sample 4. (49%NaF-38%ZrF<sub>4</sub>-12%UF<sub>4</sub>).

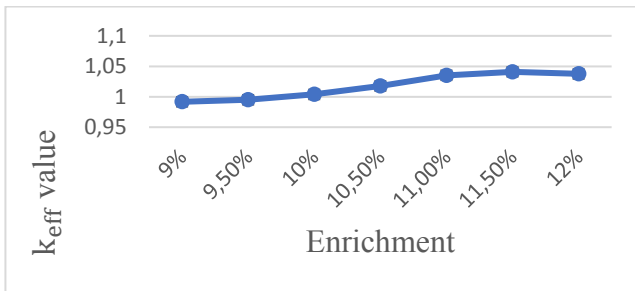


Fig. 15: Variation of  $k_{eff}$  with respect to enrichment for sample 5. (58%NaF-30%BeF<sub>2</sub>-12%UF<sub>4</sub>).

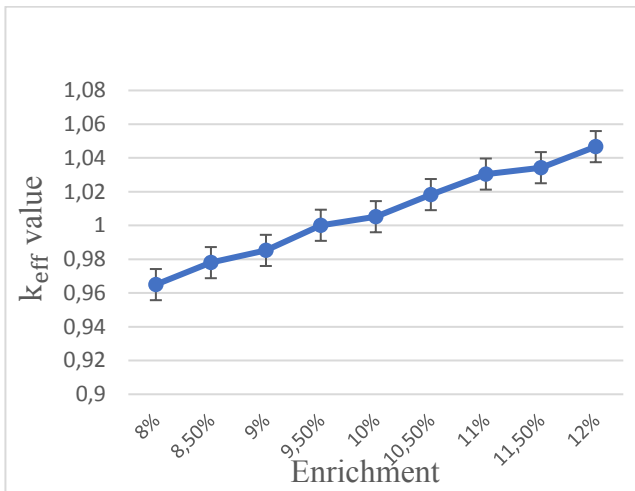


Fig. 16: Variation of  $k_{eff}$  with respect to enrichment for sample 6. (74%NaF-12%BeF<sub>2</sub>-14%UF<sub>4</sub>)

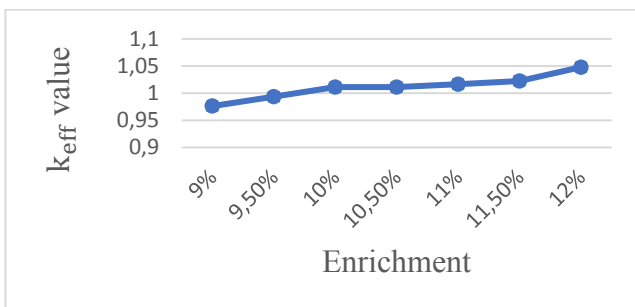


Fig. 17: Variation of  $k_{eff}$  with respect to enrichment for sample 7. (46%NaF-33%RbF-21%UF<sub>4</sub>)

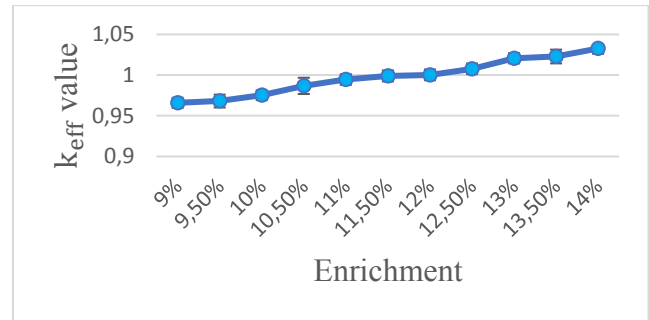


Fig. 18: Variation of  $k_{eff}$  with respect to enrichment for sample 8. (50.5%NaF-21.5%KF-28%UF<sub>4</sub>)

**Table 3:** Critical enrichment of the proposed compositions using JEFF 3.3 & ENDF/B VIII.0 data library.

Sample	Critical enrichment	$k_{eff}$ value JEFF 3.3 data library	$k_{eff}$ value (ENDF/b viii.0 data library)	Difference of $k_{eff}$ (pcm)
72%LiF-16%BeF <sub>2</sub> -12%UF <sub>4</sub>	8.5%	1.00568 ±0.00488	1.01229 ±0.00519	661
73%LiF-27%UF <sub>4</sub>	7.5%	1.00539 ±0.00413	1.00266 ±0.00360	273
78%NaF-22%UF <sub>4</sub>	10%	1.00573 ±0.00419	1.00980 ±0.00493	407
49%NaF-38%ZrF <sub>4</sub> -12%UF <sub>4</sub>	10%	1.00377 ±0.00448	1.00783 ±0.00497	406
58%NaF-30%BeF <sub>2</sub> -12%UF <sub>4</sub>	9.5%	1.00012 ±0.00444	1.00395 ±0.00475	126
74%NaF-12%BeF <sub>2</sub> -14%UF <sub>4</sub>	10%	1.0110 ±0.00512	0.99898 ±0.00564	1201
46%NaF-33%RbF-21%UF <sub>4</sub>	12%	0.99933 ±0.00484	1.00010 ±0.00594	77
50.5%NaF-21.5%KF-28%UF <sub>4</sub>	12%	1.00033 ±0.00468	1.00393 ±0.00490	360

Atom density

In MSR, atom density of U-235 in the fuel salt increases with the increase of enrichment of Uranium-235. This is because U-235 is the fissile isotope of uranium that

undergoes nuclear fission, and a higher enrichment of U-235 means that there are more U-235 atoms available for fission reactions. The higher the enrichment level, the greater the risk of a criticality accident, in which an uncontrolled chain reaction occurs. Additionally, highly enriched uranium can be used to produce nuclear weapons, so there are concerns about the proliferation of such materials. So considering all the facts that are associated, such fuel salt composition should be chosen that is comparatively better in comparison with others.

Atom density =  $(\rho \times N_A) / A$ ;  $\rho$  is the density,  $N_A$  is Avogadro's constant.

The results are shown in Table 4.

Conversion ratio (CR) and Figure of Merit (FoM)

Conversion ratio is an important parameter for choosing fuel salt compositions in molten salt reactors (MSRs) because it directly affects the overall performance and sustainability and potential for long-term operation of the reactor. The conversion ratio generally increases with decreasing U-235 enrichment in MSR. Since the FoM is dependent on the CR it also follows the same trend. Generally, the conversion ratio that is expected for MSR is less than 1 and it ranges from 0.6 to 0.9. CR & FoM are expressed by the following formulas.

$$CR = \frac{U^{238} \text{ captures}}{U^{235} \text{ captures} + U^{235} \text{ fissions}} ; FoM = \frac{CR}{\text{Enrichment}}$$

Burnup calculation of salt composition

Xenon equilibrium: As the burnup of the fuel starts in molten salt reactor, the Xenon buildup reaches to an equilibrium level. It occurs because the production of Xenon and its decay products (Cesium and Iodine) are balanced by their removal from the fuel through decay and neutron absorption. As the burnup time increases, the amount of Xenon produced in the fuel increases, leading to a decrease in reactivity due to neutron absorption by the Xenon. However, as the amount of Xenon increases, so does the rate of decay of the Xenon and its decay products. This results in an increase in the rate of neutron production, which offsets the effect of neutron absorption by the Xenon. At a certain burnup level, the production rate of Xenon and its decay products becomes equal to the removal rate, and an equilibrium condition is reached. At this point, the reactivity of the reactor stabilizes, and the Xenon poison attains equilibrium.

Fission product inventory: The inventory of Uranium, Samarium and Plutonium isotopes in the burnup of a salt composition in MSR vary depending on the specific operating conditions of the reactor. It is important to note that some of these isotopes, specifically Plutonium-239, 240, 241, and 242, have a high proliferation risk.

Table 4: Atom density at critical enrichment.

Salt compositions	Atom density (atom/cc)
72%LiF-16%BeF <sub>2</sub> -12%UF <sub>4</sub>	<b>7.81 × 10<sup>19</sup></b>
73%LiF-27%UF <sub>4</sub>	<b>1.706 × 10<sup>20</sup></b>
78%NaF-22%UF <sub>4</sub>	<b>1.73 × 10<sup>20</sup></b>
49%NaF-38%ZrF <sub>4</sub> -12%UF <sub>4</sub>	<b>9.48 × 10<sup>19</sup></b>
58%NaF-30%BeF <sub>2</sub> -12%UF <sub>4</sub>	<b>7.094 × 10<sup>19</sup></b>
74%NaF-12%BeF <sub>2</sub> -14%UF <sub>4</sub>	<b>9.34 × 10<sup>19</sup></b>
46%NaF-33%RbF <sub>2</sub> -21%UF <sub>4</sub>	<b>9.34 × 10<sup>19</sup></b>
50.5%NaF-21.5%KF-28%UF <sub>4</sub>	<b>2.82 × 10<sup>20</sup></b>

It is observed that atom density of U-235 in the fuel salt composition increase with the increase of enrichment of <sup>235</sup>U. Fig. 19 which indicate that Xenon reaches to equilibrium at about 15 days of burnup for salt composition of 73%LiF-27%UF<sub>4</sub>. Fig. 20 shows the mass of U-235 and U-238 have appeared constant for first 100 days. Sm-149 reaches an equilibrium of 1mm after 40 days of burnup. Pu -239 which is fissile nuclide having an equilibrium mass of about 10 gm & the equilibrium concentration of other isotopes of Pu are even lower. These show that the proliferation risk is negligible for this type of fuel salt compositions so this salt composition should be considered for the progress study of MSR.

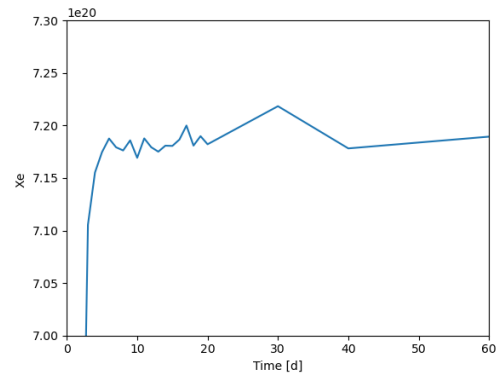


Fig. 19: Xenon equilibrium for 73%LiF-27%UF<sub>4</sub>

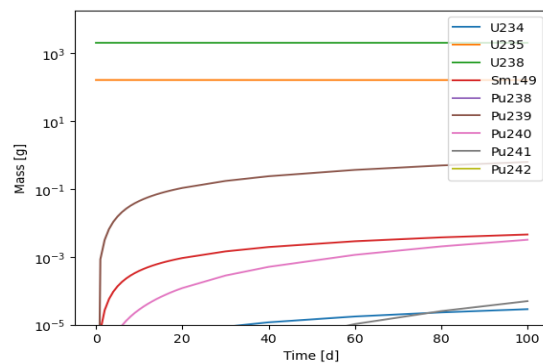


Fig. 20: Fission product inventory for 73%LiF-27%UF<sub>4</sub>

Conversion ratio (CR) & FoM

The results are shown in Table 5. It is observed for all the fuel salt compositions that they follow the increasing trend

with enrichment increasing. Since FoM is dependent on the CR they also show the same trend.

Table 5: Conversion ratio (CR) & FoM at critical enrichment

Salt compositions	CR	FoM
72%LiF-16%BeF <sub>2</sub> -12%UF <sub>4</sub>	0.9478	11.1513
73%LiF-27%UF <sub>4</sub>	0.9726	12.9680
78%NaF-22%UF <sub>4</sub>	0.8744	8.7447
49%NaF-38%ZrF <sub>4</sub> -12%UF <sub>4</sub>	0.8945	8.9451
58%NaF-30%BeF <sub>2</sub> -12%UF <sub>4</sub>	0.9191	9.6748
74%NaF-12%BeF <sub>2</sub> -14%UF <sub>4</sub>	0.8847	8.8473
46%NaF-33%RbF-21%UF <sub>4</sub>	0.8535	7.1125
50.5%NaF-21.5%KF-28%UF <sub>4</sub>	0.8649	7.2082

Temperature reactivity feedback

Temperature reactivity feedback is an important parameter for choosing fuel salt compositions in a molten salt reactor (MSR) because it has a significant impact on the safety and stability of the reactor. In an MSR, the fuel salt is both the fuel and the coolant, and it operates at high temperatures. As the temperature of the fuel salt increases, the reactivity of the reactor also increases, leading to a potentially dangerous situation if not properly controlled. To ensure the safety and stability of the reactor, it is important to select a fuel salt composition that has a negative temperature reactivity feedback.

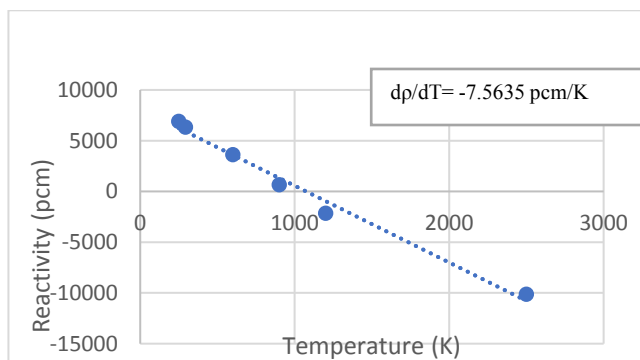


Fig. 21. 72%LiF-16%BeF<sub>2</sub>-12%UF<sub>4</sub>

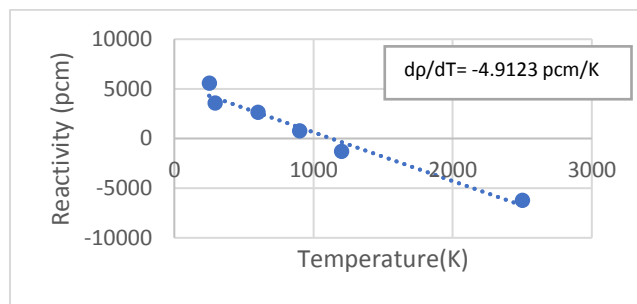


Fig. 22: 78%NaF-22%UF<sub>4</sub>.

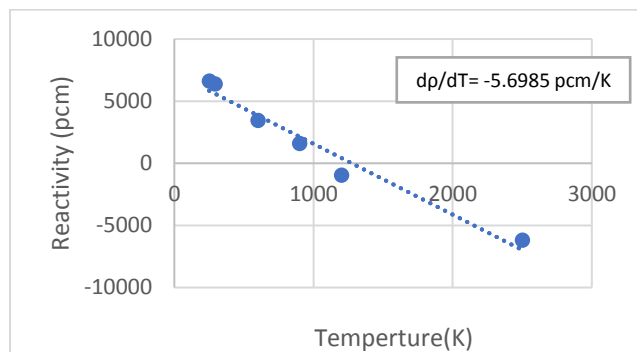


Fig. 23: 3%LiF-27%UF<sub>4</sub>

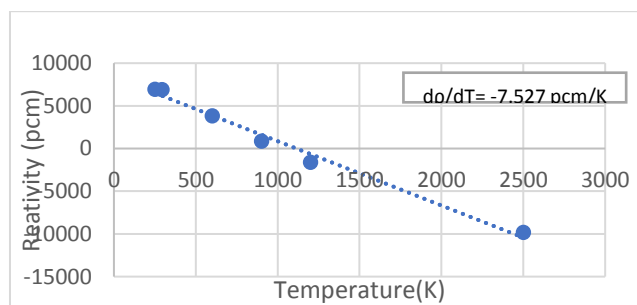


Fig. 24: 49%NaF-38%ZrF<sub>4</sub>-12%UF<sub>4</sub>

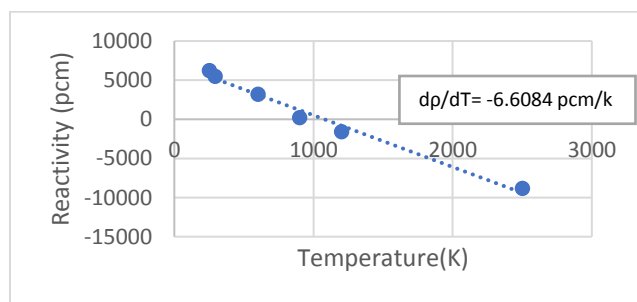


Fig. 25: 58%NaF-30%BeF<sub>2</sub>-12%UF<sub>4</sub>

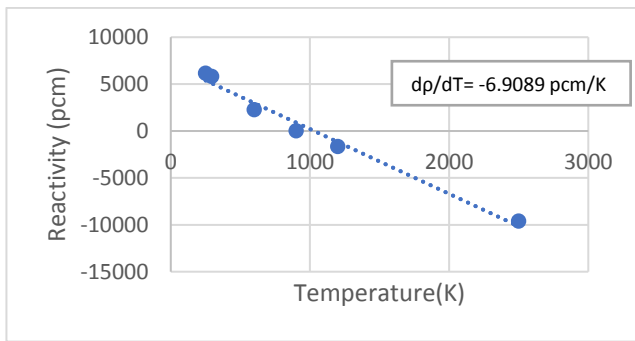


Fig. 26: 46%NaF-33%RbF-21%UF<sub>4</sub>

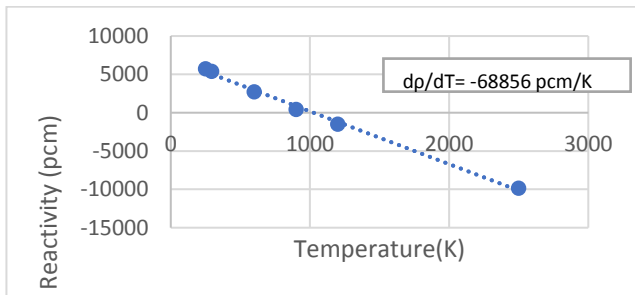


Fig. 27: 74%NaF-12%BeF<sub>2</sub>-14%UF<sub>4</sub>

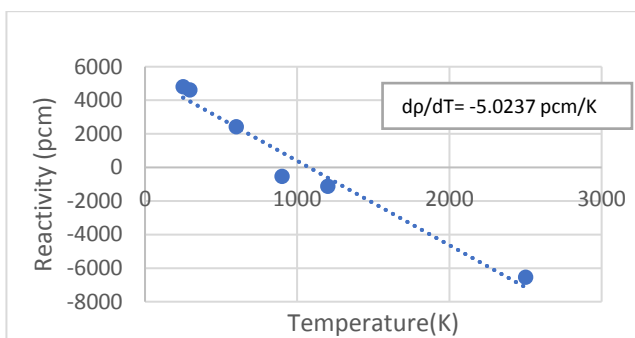


Fig. 28: 50.5%NaF-21.5%KF-28%UF<sub>4</sub>

It is observed (Figs. 21-28) that all the salt composition's temperature reactivity feedback follows the decreasing trends as of temperature increments. All the salt compositions maintain a negative temperature reactivity feedback.

### Limitations

- Lack of uncertainties in thermal scattering/bond-vibration models for molten salts (Li/Be/F) and insufficient covariance data might skew reactivity coefficients.
- Standard libraries may not adequately represent  $S(\alpha, \beta)$  for liquid salts. Graphite swelling/annealing, channel distortion, and moderation changes were idealized; nonetheless, simplistic models may underrepresent reflector leakage and bypass pathways.

### Future Work

- Coupled OpenMC with CFD/thermal solvers (e.g., Ansys, OpenFOAM/MOOSE-Moltres, Comsol) for iterative temperature-density-power fields;

- Incorporate salt viscosity/thermal expansion and graphite heat storage. Implement continuous feed/removal for Xe/Kr, noble metals, and rare earths, including residence-time distributions and precursor drift.
- Evaluate control of reactivity swing and  $\nu^-$  effects.

## 4. Conclusion

Generation IV is focused on enhancing nuclear reactor safety, sustainability, economics, and non-proliferation. MSRs are innovative GEN-IV nuclear reactors that have gained recognition recently. Although MSRs have little operating experience, considerable research on them may improve their performance. This study uses Monte-Carlo and OpenMC to examine the neutronics of a typical MSR core with varying fuel salt concentrations. Reference MSR is ORNL MSRE model. Simulations and 2-D representations display neutronic characteristics and reactor core geometry. Eight fuel salts were examined. Economic factors determine salt choices. Multiplication factors, reactivity, conversion ratio, FoM, temperature reactivity feedback, neutron spectrum, and burnup were determined. The computations use JEFF3.3 and ENDF/B VIII.0 nuclear data libraries. Fissionable and neutron poison were burned up. The neutronic evaluation of fuel salts for the ORNL molten salt reactor was performed during normal operation using OpenMC and compared to the experimental value in terms of effective multiplication factor for validation ( $K_{eff}$ ). It was 0.06%. Fuel salt's strong negative temperature reactivity coefficient makes MSRs passively safe. Consequently, the OpenMC-ORNL experimental data eigenvalue ( $K_{eff}$ ) difference is statistically ambiguous. Coolant salts like 73%NaF-27%UF<sub>4</sub> may be carrier salts due to their lower critical enrichment and higher conversion ratio. This study guides once-through molten salt reactor core design. This optimization study on molten salt reactor burnup covers more parameters than others. These findings illuminate the high-fidelity MSR concepts' end goals.

Hence, a fully connected MC-TH technique will be used to calculate depletion for the entire burnup cycle, fuel cycle length, thermal neutron flux, and fission product activity. Enrichment, moderator-to-fuel ratio, and boron content will also be examined. We will compute the essential safety parameters, such as the temperature reactivity coefficient and effectively delayed neutron fraction, to choose the scheme that meets safety requirements and maximizes economic efficiency. The topic of selecting the fuel cycle is beyond the scope of this paper, however it will be explored in future research.

LEU MSR has stable criticality and tolerable isotopic accumulation during numerous cycles. OpenMC generates accurate forecasts of neutron flux and isotope development. LEU-based MSRs can be tailored to Bangladesh's nuclear energy strategy, providing safety and sustainability benefits.

The research question, posed at the end of the Introduction, asks whether OpenMC can accurately model the complex

geometries and compositions of LEU-based molten salt reactors. This study shows that OpenMC successfully addresses this question, yielding reliable predictions of criticality, neutron flux distribution, CR and reactivity.

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### References

- [1] Renault, C, Hron, M, Konings, R, and Holcomb, D E. (2009). "The Molten Salt Reactor (MSR) in generation 4: overview and perspectives." NEA.
- [2] Jérôme Serp, Michel Allibert, Ondřej Beneš, Sylvie Delpech, Olga Feynberg, Véronique Ghetta, Daniel Heuer, David Holcomb, Victor Ignatiev, Jan Leen Kloosterman, Lelio Luzzi, Elsa Merle-Lucotte, Jan Uhlíř, Ritsuo Yoshioka, Dai Zhimin, (2014). The molten salt reactor (MSR) in generation IV: Overview and perspectives, Progress in Nuclear Energy, Volume 77, Pages 308-319, ISSN 0149-1970, <https://doi.org/10.1016/j.pnucene.2014.02.014>.
- [3] Ignatiev, V., Feynberg, O., Gnidoi, I., Merzlyakov, A., Smirnov, V., Surenkov, A., Tretiakov, I., Zakirov, R., Afonichkin, V., Bovet, A. and Subbotin, V., (2007). Progress in development of Li, Be, Na/F molten salt actinide recycler & transmuted concept. In Proceedings of ICAPP (Vol. 7, pp. 13-18).
- [4] LeBlanc, David. (2010). Molten Salt Reactors: A New Beginning for an Old Idea. Nuclear Engineering and Design. 240. 1644-1656. 10.1016/j.nucengdes.2009.12.033  
Ondřej Chvála., (2014). Proceedings of ICAPP 2014 Charlotte, USA, Paper 14187
- [5] Ignatiev, V.V., Feynberg, O.S., Zagnitko, A.V., Merzlyakov, A.V., Surenkov, A.I., Panov, A.V., Subbotin, V.G., Afonichkin, V.K., Khokhlov, V.A. and Kormilitsyn, M.V. (2012). Molten-salt reactors: new possibilities, problems and solutions. Atomic energy, 112, pp.157-165.
- [6] R. C. ROBERTSON, "MSRE Design and Operations Report Part I: Description of Reactor Design," ORNL-TM-0728," Oak Ridge National Laboratory (1965).
- [7] Dan Shen,<sup>a</sup> Germina Ilas,<sup>b</sup> Jeffrey J. Powers,<sup>b</sup> and Massimiliano Fratoni, Reactor Physics Benchmark of the First Criticality in the Molten Salt Reactor Experiment, Nuclear Science and Engineering, Vol. 195, 825-837, 2021, DOI: <https://doi.org/10.1080/00295639.2021.1880850>
- [8] Thoma, R. E. (Ed.). (1959). Phase diagrams of nuclear reactor materials (Vol. 2548). Oak Ridge National Laboratory.
- [9] Thoma, R. E. (1968). CHEMICAL FEASIBILITY OF FUELING MOLTEN SALT REACTORS WITH PuF (No. ORNL-TM-2256). Oak Ridge National Lab., Tenn.
- [10] Cantor, S. (1968). PHYSICAL PROPERTIES OF MOLTEN-SALT REACTOR FUEL, COOLANT, AND FLUSH SALTS (No. ORNL-TM-2316). Oak Ridge National Lab., Tenn.
- [11] Briggs, R.B., (1966). Molten-Salt Reactor Program, Semiannual Progress Report For Period Ending February 28, 1966, ORNL-3936, ORNL.
- [12] Williams, D. F., Toth, L. M., and UT-Battelle, L. L. C. (2005). Chemical considerations for the selection of the coolant for the Advanced High-Temperature Reactor. ORNL/GEN4/LTR-05-011, Oak Ridge National Laboratory, Oak Ridge, TN.

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