



## Parametric study of thermal molten salt reactor neutronics criticality behavior



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### ABSTRACT

The molten salt reactor (MSR) research and development has attracted more attention recently. Various concepts of MSR designs have been proposed, and related researches regarding MSR materials technologies, neutronics behavior, thermal-hydraulic behavior and the reactor safety have been reported. The MSR neutronics criticality behavior has significant effect in the MSR research aspect. It is important to conduct the comprehensive and systematic investigation of thermal MSR neutronics criticality behavior. In this work, the molten salt reactor type that molten salt dissolves the fuel materials is investigated. Therefore, the evaluations of different thermal MSR neutronics criticality behavior are conducted in this work. By far, various molten salt fuel types have been proposed by different research institutes based on different considerations. Consequently, the evaluation on neutronics characteristics of different molten salt fuel types and the parametric study of neutronics behavior are taken into account. Furthermore, some molten salt fuels contain the lithium element with the isotope Li-6, which has a large thermal neutron absorption cross section. The evaluation of different Li-6 concentration effects is also considered in this work. In addition to the fuel and moderators effect, other parameters such as the volume and geometry effects are also studied. Lastly, the operation temperature on the neutronics behavior is also investigated. The corresponding parameters such as multiplication factor, neutron spectrum, and temperature coefficient are evaluated. In this work, instead of the simulation of whole reactor core, the simulation of a thermal MSR fuel unit is conducted. This work provides a more complete and comprehensive evaluation approach for various parametric effect on MSR neutronics criticality behavior and offers reference for the MSR criticality design.

### 1. Introduction

The fission products could poison fuel and reduce  $k_{\text{inf}}$ . Therefore, on-line refueling or the fission product removal process during the operation could increase the sustainability. Combined with the possibility of on-line removal of fission products and on-line refueling, the molten salt reactor (MSR) has the advantage of transmuting fertile material (such as thorium) to fissile material, which makes MSR as one of the most sustainable Generation IV reactors up to now. MSR has the advantages of higher operation temperature and almost operated at atmospheric pressure. There are two types of MSR. For one type, the molten salt dissolves the fuel materials and the molten salt acts as both fuel and coolant. For such kind of MSR concept, both fast spectrum MSR concepts and thermal spectrum concepts have been investigated up to now. In the fast spectrum MSR concepts aspect, the designs, such as Molten Salt Fast Reactor (MSFR) and MOlten Salt Actinide Recycler & Transmuter (MOSART), have been proposed. In the thermal spectrum MSR concepts aspect, the designs, such as MSBR (Molten Salt Breeder

Reactor) and MSR-FUJI, have been proposed. In the molten salt selection aspect, mainly fluoride salt and chloride salt are used. For another type, the fuel material is made of coated particle and the molten salt just acts as the coolant. The first type of MSR is considered in this work. The research topics, such as salts and materials, fuel and fuel cycle, design and operation, are the technical issues and priorities for the MSR technology development, and the MSR neutronics study has significant and fundamental effect for the MSR research improvement (Serp et al., 2014). It is important to conduct the comprehensive and systematic investigation of thermal MSR neutronics criticality behavior. Therefore, the parametric study of thermal molten salt reactor neutronics criticality behavior needs to be carried out.

Up to now, various molten salt fuel types have been proposed and studied. Besides, some molten salt fuels contain the element of lithium. For the natural lithium, it contains the Li-6, which has significant larger cross section compared to Li-7 in the thermal and epithermal energy region. Up to now, although graphite is widely used as the moderator for molten salt reactor, but other material such as BeO can also be used

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as the moderator. Besides the fuel and moderator compositions effect, other parameters such as the volume and geometry effect are also studied. In detail, the cuboid, cylindrical and hexprism types of geometries are studied. In addition to the molten fuel compositions and geometry study, the temperature effect is also studied (Robertson, 1971; Nagy et al., 2008; Yu et al., 2017; Li et al., 2017; Si et al., 2017). In a nutshell, various aspects such as different molten salt fuel types, different fuel unit geometries and different moderators are evaluated in this work. This work provides more comprehensive and systematic evaluation work for different parameters effect on MSR neutronics criticality behavior.

## 2. Parameter study of molten salt reactor neutronics criticality behavior

The neutronics criticality design of MSR comprises many aspects such as the selection of molten salt fuel materials, the molten salt fuel operating temperature, the molten salt fuel concentrations, the selection of moderators, the moderator density, and geometry type and geometry size. In general, this work has been performed to discuss how these parameters would affect the MSR thermal reactor criticality behavior.

SCALE 6.1 has been used for the thermal MSR neutronics criticality behavior evaluation in this work. In detail, the CSAS6 (Criticality Safety Analysis Sequence with KENO-VI) in SCALE 6.1 is used. The neutronics criticality behavior in the thermal MSR fuel unit is simulated by the Monte Carlo method in the KENO-VI model (ORNL, 2011).

In order to evaluate various parameters effect on the thermal MSR neutronics criticality behavior quantitatively, a simple base case has been built and used for comparison. The schematic of geometry of base case in SCALE 6.1 is shown in Fig. 1, and the main boundary conditions of base case is shown in Table 1. Regarding the physical properties of molten salts, various research in the experimental and review aspects has been conducted, such as the work conducted by Romatoski and Hu (2017). The physical properties of molten salt and graphite used in this work refer to the MSBR design (Robertson, 1971). Besides, the reflective boundary condition is used in the simulation in this work. For the graphite, the 'c' nuclear data in the current code package is used. The main effect of molten salt fuel circulation behavior on the reactor criticality behavior is the movement of delayed-neutron precursor, which could cause the decrease of k-inf value. Up to now, various research on the delayed-neutron precursor effect has been conducted, such as the work conducted by (Zhang et al., 2009a, 2009b) in which both the effect of delayed-neutron precursor circulation on the steady state and transient state were investigated. In the current work, the criticality behavior of fresh molten salt fuel, which means there is no delayed-neutron precursor at current moment, is investigated. Besides, once the molten salt fuel undergoes the burnup behavior, the delayed-neutron precursors will be generated by the fission behavior, and the effect of molten salt fuel circulation behavior on the criticality behavior and reactor control should be considered.

### 2.1. The criticality behavior of different fuel materials

Up to now, various molten salt fuel types can be used for the MSR designs, the evaluation of these materials criticality behavior is considered. First, the evaluation of different molten fuel salts criticality behavior is evaluated. Second, the effect of different U-233, U-235 and Pu-239 concentrations is evaluated. Third, the Li-6 concentration effect on the criticality behavior is investigated.

#### 2.1.1. The effect of different fuel compositions

In this work the neutronics characteristics behavior of the following molten fuel salts is evaluated. In details, the molten fuel salts of LiF-BeF<sub>2</sub>-ZrF<sub>4</sub> (64.5-30.5-5 mole %), LiF-NaF-BeF<sub>2</sub> (31-31-38 mole %), LiF-NaF-ZrF<sub>4</sub> (42-29-29 mole %), LiF-ZrF<sub>4</sub> (51-49 mole %), LiF-RbF (44-56

mole %), NaF-BeF<sub>2</sub> (57-43 mole %), NaF-ZrF<sub>4</sub> (59.5-40.5 mole %), RbF-ZrF<sub>4</sub> (58-42 mole %), and LiF-NaF-KF (46.5-11.5-42 mole %) neutronics criticality behavior is evaluated (Nagy et al., 2008; Yu et al., 2017). In the fuel salt setting aspect, the same fuel atom density of the base case is applied. In detail, for each case, 12 mole % of ThF<sub>4</sub> and 0.3 mole % of UF<sub>4</sub> are applied, and for the rest of the fuel mole fraction, different molten fuel salts with its corresponding components are applied in each case.

Fig. 2 shows the k-inf values for different fuel salts with different side lengths by SCALE 6.1 (CE). It can be seen that the molten salts have Li-7 and Be-9 isotopes would have better neutronics criticality characteristics. This is mainly because that for these molten salts, the Li-7 and Be-9 isotopes have better neutron moderation ability than other isotopes. Besides, the k-inf values vary with the change of half side lengths. For the condition of that the half side length is 9 cm, the k-inf values reach the highest value among these different side lengths for most of the cases. Generally, for the molten salt that has higher k-inf values at one half side length, it would also have higher k-inf value at other half side length, except for some specific cases. For the condition that the value of k-inf is less than or close to 1.0, it could not be treated as the possible design configuration for the whole core.

Fig. 3 shows the normalized neutron flux per unit lethargy with neutron energy for different molten salt types at 6 cm half side length condition. Three different fuel salts: A (base case), B (LiF-NaF-KF) and C (RbF-ZrF<sub>4</sub>) are selected for comparison. No matter in the fuel region and moderator region, material type A has more thermal and epithermal neutron fraction than other two cases, which is mainly because for material type A, it has more Li-7 and Be-9 atom density, which could have better moderation ability.

#### 2.1.2. Different concentrations of fuel materials

The fissile isotopes such as U-233, U-235 and Pu-239 could be acted as the fuel materials in the molten salt. For example, U-233 could be used for U-Th cycle. For the type of MSR investigated in this work, the continuously on-line fission products removal and on-line fuel material adding are possible. For example, the fission products, such as the fission gases, can be removed. In the MSR, the U-233 can be used as the fuel with Th-232, due to fertile material of Th-232 can be transmuted to fissile material of U-233. Besides, the Pu-239 can be used as the fuel with U-238, due to U-238 can be transmuted to Pu-239. Therefore, different fuel material neutronics behavior is evaluated and different fuel isotopes concentration effect is also investigated.

The base case is applied here, but the fuel isotopes varied with different cases and different half side lengths are considered. In detail, different concentrations of fuel isotopes are assumed and applied for different cases, and the ratio of U-233, U-235 and Pu-239 means the atom density of these cases compared with the atom density of the base case, and other isotopes atom densities do not change. The effect of different fuel isotope concentration on the criticality behavior is investigated. In the current work, the burnup effect is not considered.

Fig. 4 shows k-inf for different fuel isotopes concentrations with different half side lengths by SCALE 6.1 (CE). It can be seen that no matter for which case, at the same fuel isotope concentration condition and same half side length, k-inf values for the cases of U-233 and Pu-239 are generally higher than U-235. For the U-233 case and Pu-239 case, the higher k-inf values vary with different fuel isotopes concentrations and half side lengths. For example, for the case of that the half side length is 6 cm, the k-inf of the case with Pu-239 is higher than the case with U-233 in the beginning, and then becomes smaller than the case with U-233. Fig. 5 shows the k-inf for U-233 at different side lengths with different concentrations by SCALE 6.1 (CE). At one certain fixed U-233 concentration, no matter for which case it can be seen that when the half side length is 9 cm the k-inf reaches the highest value. From Fig. 5, it is also clearly that under smaller half side length condition, the system is under-moderated, and while under the larger half side length condition, the system is over-moderated. The highest k-inf

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