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Modeling and criticality calculation of the Molten Salt Fast Reactor using Serpent code

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Abstract. In Molten Salt Fast Reactors (MSFR), a liquid-fuel circulates through the cylinder core and transport the fission heat to the Intermediate external Heat Exchangers (IHX), therefore liquid salt allows carrying the fuel and transfer heat. The MSFR supposed to work in a closed Th-based fuel cycle with a full reprocessing of fission products and all actinides in the core. The aim of this paper is; modeling the primary circuit of the MSFR (based on the European model) in order to identify the composition of the start-up fuel required to the criticality. In conclusion, the compositions of the start-up liquid fuel required for criticality and long life cycle were determined precisely for three different types of fissile materials ($^{233}\text{UF}_4$, PuF_3 and TRUF_3).

Keywords: molten salt fast reactor; thorium fuel cycles; fast neutron spectrums.

Highlights:

- Modeling of the primary circuit of the MSFR
- Optimize the composition of fissile material in start-up fuel.

Acronyms:

MSR	Molten Salt Reactor
MSFR	Molten Salt Fast Reactor
TRUs	TRansUranic isotopes
ORNL	Oak Ridge National Laboratory
FPS	Fission Products
MAs	Minor Actinides
GIF-IV	The Generation IV International Forum
AR	Advanced Reactor systems
MOSART	MOLten Salt Actinide Recycler and Transmuter
EVOL	Evaluation and Viability Of Liquid fuel fast reactor system
SAMOFAR	Safety Assessment Of the Molten Salt Fast Reactor
LWR	Light Water Reactor
PUREX	reprocessing technique
NPP	Nuclear Power Plant
EFPD	Effective Full power days



1. Introduction

The Molten salt reactors (MSRs) are a group of fission reactor concepts which deals with the fuel as a liquid. Such types of reactors expected to operate using molten salts as a fuel. Some advantages of liquid-fuelled reactors are [1]:

- Online reprocessing and adjustment of fuel composition during reactor operation;
- Heat produced directly in the heat transfer fluid;
- Absence of the difficulties of solid fuel fabrication with large amounts of TRansUranic isotopes (TRUs) can be overcome using MSRs;
- Maximum utilization of resources and homogeneity of the fuel [1];
- Possibility to reconfigure the geometry of the fuel passively, for example, by the effect of gravity.

In the 1950s, effective experimental studies were done at Oak Ridge National Laboratory (ORNL), providing an experimental basis for MSRs feasibility. In 1958 liquid fuel based on water was used in a 5 MWth homogeneous reactor experiment called HRE-2, illustrating the intrinsic stability of homogeneous reactors. Subsequently, the Molten Salt Reactor Experiment [2,3,4]. The results showed the possibility of circulating a liquid fluoride mixture without significant corrosion problems. This was achieved by using nickel-based alloy (Hastelloy N) and oxidation control of the fuel by use of the U^{3+}/U^{4+} buffer. However, this 8-MWth thermal reactor only tested fissile isotopes (^{233}U , ^{235}U , Pu) and not fertile ones such as Th because it was not intended to operate as a breeder reactor but as an experiment. Nevertheless, a continuous physical processing of the fuel was successfully tested, consisting in contacting the fuel with a neutral gas to extract gaseous fission products (FPs) [1]. Despite this success, these tests (studied in detail by ORNL) did not lead to the construction of the Molten Salt Breeder Reactor [5,6]; partly because its thermal spectrum requires intensive chemical processing for FP removal and Pa extraction. In general, FP removals were designed for this reactor because the thermal spectrum design benefits greatly from the removal of specific absorber elements, this increases fuel cycle performance. Using a fast spectrum can limit the intensive chemical processing [1]. The MSR has been selected by the Generation Four International Forum (GIF-IV) in 2001 as one of the six advanced reactor systems (AR) for further research and development. Later on, two fast-spectrum MSR designs are being studied [7,8,9,10], both of them are based on the fast-spectrum, Th-based fuel and liquid fuel circulation: MSFR concept essentially developed at CNRS, France, and the Molten Salt Actinide Recycler and Transmuter (MOSART) concept under development in the Russian Federation. MSFR concepts supposed to match the technology goals of the GIF: sustainability, economics, safety and reliability, and proliferation resistance and physical protection [11].

The MSFR developed essentially by the EURATOM EVOL (Evaluation and Viability Of Liquid fuel fast reactor system) Project [12]. Different and prospective studies ongoing nowadays to investigate that fast-spectrum MSR systems satisfy the goals of GIF. Currently, the SAMOFAR project (Safety Assessment Of the Molten Salt Fast Reactor) seeks to improve and develop the main achievements of the preceding EVOL project, and consequently further steps towards the industrial implementation of MSFR.

MSFR supposed to simplify the reactor core by using molten salt mixture fluid which works as a coolant and fuel simultaneously. In other words, fissile material is dissolved in the molten salt and circulated through the core. This is a clear advantage of MSFR over the conventional nuclear reactors. MSFR conceived to operate under ambient pressures and high outlet temperatures. The ability to online remove of FPs and add fissile and/or fertile material. As a result of online reprocessing, MSFR has comparatively low excess reactivity, high burnup, low waste production, and high capacity factors. Furthermore, the breeding capabilities conceived to be enhanced by using the molten salt breeding blankets which surrounding the core radially.

Indeed, there are challenges that obstacles commercial adoption of MSFR. For example, identifying structure materials which can withstand the corrosive, high-temperature and high-flux environment of the primary circuit. Avoiding salt freezing in delicate components and melt frozen salt

elsewhere. Proliferation legitimate concerns related to breeding blankets that can be used to produce weapons. Moreover, the characteristics of MSFR introduce computational challenges in accurately predicting dynamic manner [13]. Due to the lack of detailed data about the optimal concentration and type of the loading fuel for MSFR, authors want to determine accurately the optimum composition of the start-up liquid fuel.

The aim of this paper is; modeling the primary circuit of the MSFR (based on the European model) in order to identify the composition of the start-up fuel required for criticality and long life cycle.

The paper is organized as follows; after a general introduction about the MSR systems, section 2 including also a brief presentation of the European reference MSFR, section 3 focuses on the methodology and tools, which used in this work. Finally, the main results related to fuel concentration calculations are discussed in section 4. The main conclusion is drawn in section 5.

2. Materials and Methods

In MSFR the fuel is expected to dissolve in a LiF salt, which plays also the role of the coolant [14]. Thermal power of MSFR is 3000 MW with a fast neutron spectrum, while the average power density is 48.6 MW/t-HM [14]. Thermal efficiency about 50%, the expected inlet temperature is 650 °C, while the outlet is 750 °C [14,16]. In the MSFR, a liquid fuel salt circulates through the core and transfers the heat to 16 external heat exchangers, and then through the pumps, it re-enters at the bottom of the core. The core geometry can be assumed as a cylindrical vessel with diameter and height of 2.25 m made of a nickel-based alloy filled with the fuel [17]. MSFR operate under ambient pressure. Figure 1 shows the schematic structure of the MSFR.

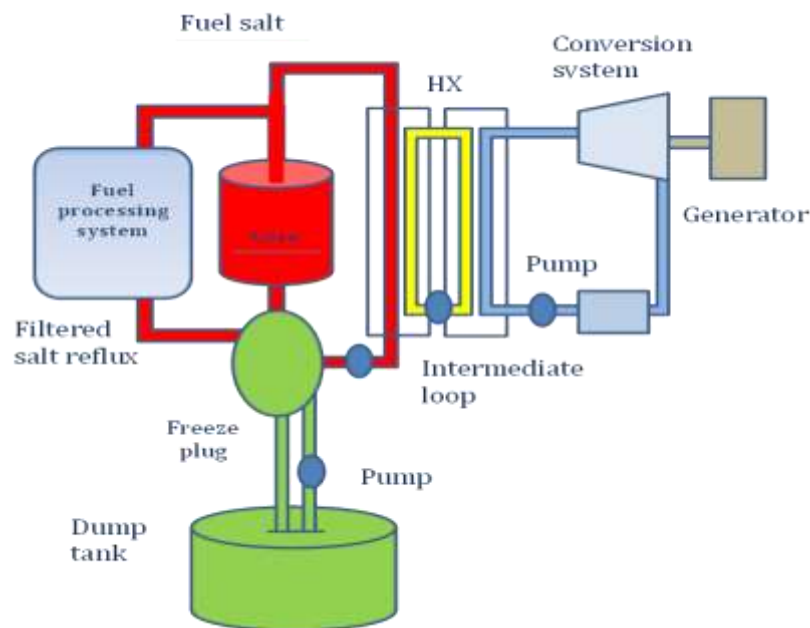


Figure 1. The schematic structure of the MSFR.

2.1. Start-up core loadings

The fuel salt is composed of LiF for 77.5 mol%, and by a mixture of AcF_3 and AcF_4 for 22.5% (Ac indicates actinides). The fuel salt volume is 18 m³ in total in the primary circuit. Three fuel compositions have been considered in this work; Th- U^{233} , Th-Pu, and Th-TRU (TRU is TRansUranic).

In the first case, i.e. using Th- U^{233} , it would minimize the transition time to the equilibrium cycle. In the future, the U^{233} can easily produce from MSFR (i.e. breeding reactors), but in order to overcome the unavailability of U^{233} different fissile material can be used instead of U^{233} . For example, the

second case, Th-Pu core is composed by Th and Pu, presumably from Light Water Reactor (LWR) used fuel reprocessing. Th-Pu start-up fuel appears to be more realistic because it would employ the current PUREX reprocessing technique and facilities to recover an already available fissile resource; the MSFR would then initially operate as a Pu burner [18]. Finally, The MSFR supposed to be used as a burner of the entire TRU vector produced by the LWR fleet, while initiating a new Th cycle [12]. In this case, Th-TRU with 5-year cooled TRU from LWR used fuel would be the pursued option [18].

The core is surrounded radially by a container filled with a blanket salt containing thorium to increase the breeding gain. The composition of blankets is LiF-ThF₄ (77.5 mol% LiF and 22.5 mol% ThF₄ for all cases considered).

Surrounding the blanket a 20 cm thick B₄C layer is planned to use, which can protect the heat exchanger from the neutrons. Above and below the core, 1m thick nickel-based alloy reflectors are present in order to improve neutron economy [19]. The density of the fuel salt is 4.1g/cm³ [16]. The NPP includes three different circuits involved in order to generate power: the fuel circuit, the intermediate circuit, and the power conversion circuit. These circuits are associated with other systems composing the whole NPP, such as online reprocessing units and the emergency draining system (see Figure 1).

3. Methodology and tools

Current neutron transport tools are designed to deal with the solid-fueled reactors, therefore the modeling of liquid-fueled systems have many challenges. Two main challenges are presented by liquid-fueled systems: (1) flowing of the liquid salt and (2) online reprocessing system [20]. From a modeling point of view, the axial-symmetric representation of the core can be extended to the entire primary circuit by approximating the 16 external loops with a single annular loop [18]. In this work, two dimensional (2D) axial-symmetric representation of the MSFR has been modeled with neglecting the online fuel reprocessing. The present paper investigates the MSFR neutronics by determining the concentration of fissile material required for criticality. Serpent code has been adopted, following the need for an accurate determination of these quantities. Serpent is a three-dimensional continuous energy Monte Carlo neutron transport and burnup code. The results were obtained after full-core runs of 10 million active neutron histories with the version 2.1.29 of the code. Simulations consisted in 500 active cycles of $2 \cdot 10^4$ neutrons. 20 inactive cycles were used for the convergence of the fission source distribution.

4. Results and discussion

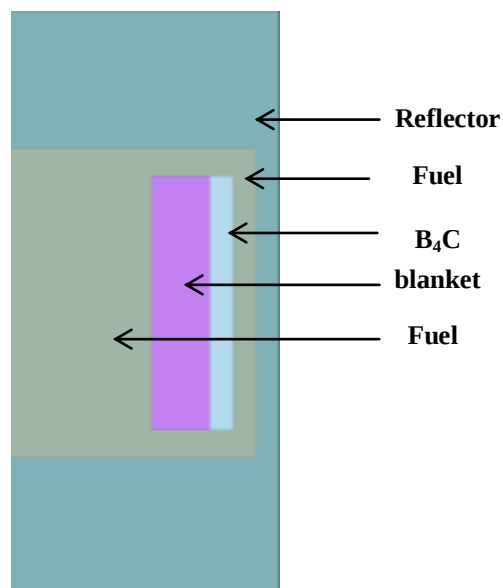
A simplified model of a MSFR primary circuit has been performed with neglecting the online fuel reprocessing. The fissile material was Th-U²³³, Th-Pu and Th-TRU Table 1. The input model from Monte Carlo code ‘Serpent 2.1.29 adopting the ENDF/B-VII library’ illustrated in the Figure 2.

The liquid fuel salt was considered as a homogeneous material. The infinite multiplication factor as a function of the concentration of fissile materials demonstrated in the Figure 3. One can notice that in the case of ²³³UF₄ the concentration should be equal to 3 mol%, this concentration corresponding to $K_{\infty}=1.07132 \pm 0.00045$ (see Figure 3). But in the case of PuF₃ as a fissile material, the concentration should be equal to 6 mol%, this concentration corresponding to $K_{\infty}=1.05407 \pm 0.00048$. Finally, for TRUF₃ the concentration should be equal to 6.5 mol%, this concentration corresponding to $K_{\infty}=1.02713 \pm 0.00043$. Although there is a good agreement between our results and results in [19] in the case of TRUF₃ and ²³³UF₄, the comparison for the PuF₃ case not held due to the lack of data.

It is known that the effect of ¹³⁵Xe and ¹⁴⁹Sm is more significant in the MSFR than in the other fast systems because the neutron spectrum is softer in the MSFR [15]. Therefore, Xenon should be removed during an operation of the molten salt reactor systems, as having gas entrained within the fuel salt presents major issues.

Table 1. The proportions of the Transuranic elements.

Isotope	Proportion of the mix (Vol%)
^{237}Np	6.3%
^{238}Pu	2.7%
^{239}Pu	45.9%
^{240}Pu	21.5%
^{241}Pu	10.7%
^{242}Pu	6.7%
^{241}Am	3.4%
^{243}Am	1.9%
^{244}Cm	0.8%
^{245}Cm	0.1%
Total	100%

**Figure 2.** Simplified axial symmetric geometry adopted in the Monte Carlo simulations.

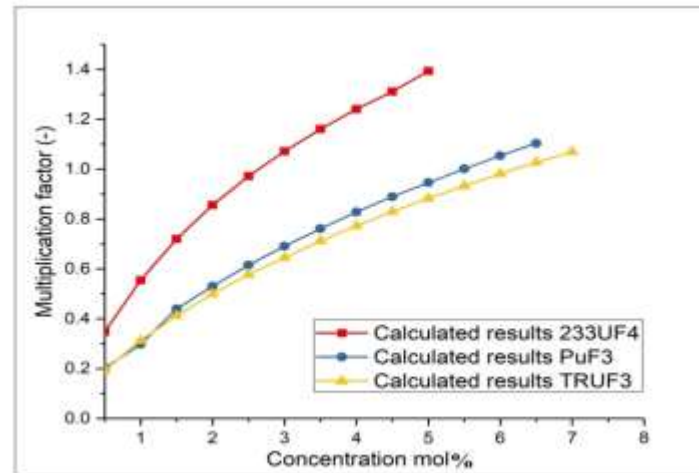


Figure 3. The infinite multiplication factor as a function of the concentration of fissile materials.

According to the Figure 4, one can notice that ^{135}Xe and ^{149}Sm have higher absorption cross-sections of lower neutron energy [21]. The optimum compositions of start-up liquid salts were; LiF 77.5 mol%, ThF₄ 19.5 mol% and $^{233}\text{UF}_4$ 3 mol% or LiF 77.5 mol%, ThF₄ 16.5 mol% and PuF₃ 6 mol% or LiF 77.5 mol%, ThF₄ 16 mol% and TRUF₃ 6.5 mol% respectively. It is worth noting that, for the determination of the accurate value of the multiplication factor, it is necessary to take into account the circulation of the fuel salt through the core [15].

5. Conclusion

A simplified model of a MSFR primary circuit has been elaborated. Calculations using Monte Carlo code Serpent 2.1.29 adopting the ENDF/B-VII library has been performed in order to determine the optimum composition of the start-up liquid fuel required for criticality and long life cycle. According to the obtained results the compositions were 3 mol% of $^{233}\text{UF}_4$, 6 mol% of PuF₃ and 6.5 mol% of TRUF₃ respectively. Effective online reprocessing and refueling system is required during burnup calculation in order to keep the reactor critical for the long life cycle.

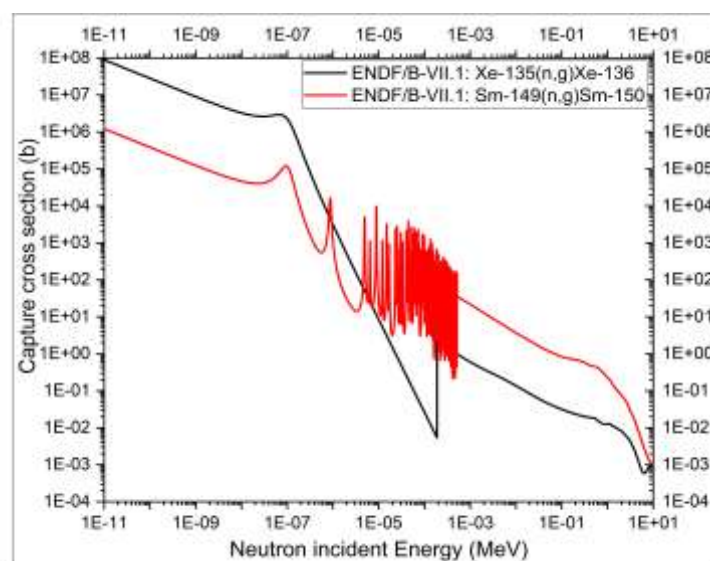


Figure 4. The cross-section of ^{135}Xe and ^{149}Sm .

Conflict of interest

The authors declare no conflict of interest.

Acknowledgements

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