ANALYSIS OF VARIOUS CANDIDATE SALTS FOR MOLTEN SALT REACTOR APPLICATION BY MCNP SOFTWARE

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Abstract: In present study, the model of Molten Salt Reactor was developed for Monte Carlo N-Particle Transport [1] computational code analysis. In the course of work, two main tasks were fulfilled, which are simulation of target material behavior as a neutron convertor (producer) under 800MeV energy proton beam and criticality calculation of the designed reactor. As a result of analysis through the MCNP software, neutron flux, as well as the value of k_{eff} multiplication factor of Molten Salt Reactor for a number of different molten salts compositions assessed.

Keywords: Molten Salt Reactor, MCNP, criticality, Thorium

1 INTRODUCTION

Being the ones investigated in the past [2], molten salt reactors presents increasing interest nowadays due to various advantages, such as low excess reactivity, low pressure, attractive $Th-U$ fuel cycle, etc. For this kind of reactors nuclear fuel is in the phase of liquid and continuously circulated through the core. The advantage of such reactors is the capability of use with accelerator, which opens the way of consumption of abundant Thorium as a nuclear fuel. The thorium fuel cycle is dependent on the conversion of the fertile isotope ^{232}Th to the fissile isotope ^{233}U, an isotope that is not found in nature, which leads to a significant engineering challenge. Reactor internals consists of the lead target placed in the central part of the vessel, the beam pathway designed for irradiation of the target, graphite layers for neutron moderation and holes through them as fuel channels. It is proposed that fuel, in a liquid phase must flow through the reactor vessel providing heat to the exchanger and enter back to the reactor from the bottom. As a fuel, thorium should be used with additional salt composition. But thorium as is not a fissile material but fertile, capable to produce ^{233}U isotopes when absorbs the neutron. Conversion should be achieved by accelerator with 800 MeV proton beam, directed from the top of the system to the lead target [3]. Lead plays a role of neutron convertor, which will produce sufficient amount of neutrons to sustain the $Th-U$ fuel cycle. The reactor should operate at a temperature of about 700 degrees Celsius. According to design, the multlipication factor of the system should be about 0.95 compared to $\boldsymbol{k_{eff}} = 1$ for a classical reactor. However, by making up for the 5-10 % loss of neutrons from an external neutron source, the system would function effectively even though the chain reaction would not be self-sustaining.

In the current study, the base for the Molten Salt Reactor was taken from the work of C. Bownman [3]. According to its data, reactor vessel is a 5 m tall cylinder with a diameter of 4 m. Beam pathway length is 2.15 m with a diameter of 0.2 m. Proton beam should be directed through this path to irradiate lead target with a dimentions of 0.7 m and 0.2 m for length and diameter respectivley.

2 MCNP SIMULATION

Two separate tasks were performed for Molten Salt Reactor investigation, however same model used for both cases with same material compositions. The first one was concentrated on the simulation of spallation target under 800MeV energy proton beam to calculate the neutron flux and energy distribution and the second one was the assessment of k_{eff} for a several molten salt fuel compositions[4]. Since the quantity and dimensions of fuel channels are not provided, it was chosen to model 50 channels with a radius of 10 cm distributed throughout the core (Figure 1). Simulation tasks were conducted under default CEM03.03[5] physics model. As a result of interaction of protons with the lead target neutrons should be produced, which themselves should make fertile ^{232}Th produce fissile ^{233}U. Run was done with 1.0E+6 particle histories on the "nps" card.

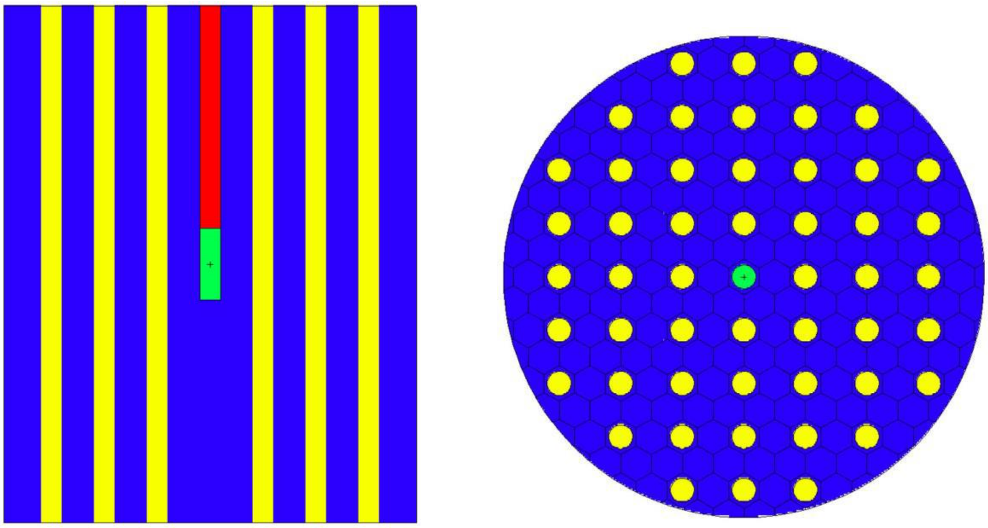

Figure 1: Molten Salt Reactor Core (vertical and horizontal cross sections), Blue – Graphite, Yellow – Molten Fuel, Red – Beam Pathway, Green – Lead Target

For the second task, as initial condition for energy distribution of neutrons source for the criticality calculation the outcome from the first simulation was used. In such a way, neutrons were modeled in all the fuel channels in the central horizontal plane of the system with the same energy distribution as the starting source for thorium cycle. For criticality calculation the same "kcode" card values were used for all investigated salts compositions, which are: 10000 neutrons the number of sources per cycle, 1.0 as a value for initial guess of k_{eff}, 200 numbers of cycles to be skipped before beginning tally accumulation and 600 as a total number of cycles to be done. For thermal treating a free-gas model was involved. Cross Section for graphite moderator from $S(\alpha,\beta)$ libraries [6] has been set appropriate to the temperature of normal operation on "mt" card of the input file. According to design, a 500-MWt thermal ADEP (Accelerator-Driven Energy Production) system can be brought into power production by a start-up inventory of 10,000 kg of Th and 700 kg of 20 % low enriched uranium. However, the ratio between fuel and salt addition is not provided, but was obtained as a separate task by the MCNP software with a condition of getting a result of about 0.95 for the multiplication factor, as preposed in the reference [3]. Doing so, 80% to 20% weight ratio between fuel and salt was assessed for further simulations. For cross-section data, those appropriate for operational temperature of the reactor were chosen. Nuclear data libraries used in simulations are presented in the Table 1. Alongside with nuclear fuel ^{232}Th ^{233}U a number of different fluorides, chlorides, nitrides salt compositions were simulated with 20% in composition. Furthermore, neutron fluxes and energy deposition inside the core were shown using the "tmesh" card. All MCNP runs for the second task were done with more than 6.0E+6 particle histories.

Library	Material
ENDF70/A	nat. C, N, O, Ar, Ar, Ar, F, Na
ENDF70/I	206Pb, 207Pb, 208Pb
ENDF70/K	232Th
ENDF70/J	233U
ENDF71/X	nat. Rb, Na, Be, Li, Cl, Zr, K, Ca

Table1: Nuclear Data Libraries

3 RESULTS OF ANALYSIS

1) LEAD TARGET IRRADIATION

The results of neutron flux calculation for 800MeV energy proton beam irradiation are shown in figure 2 with an average relative error value of 0.018%. The neutron flux values were divided into energy bins ranging from 1E-8 to 15 MeV. It is well seen from the graph that neutrons with energies up to 0.01keV are greater in contrast to the neutrons with higher energies. Total neutron production per source particle was calculated 16.14 n/p with a relative uncertainty of 0.0013%.

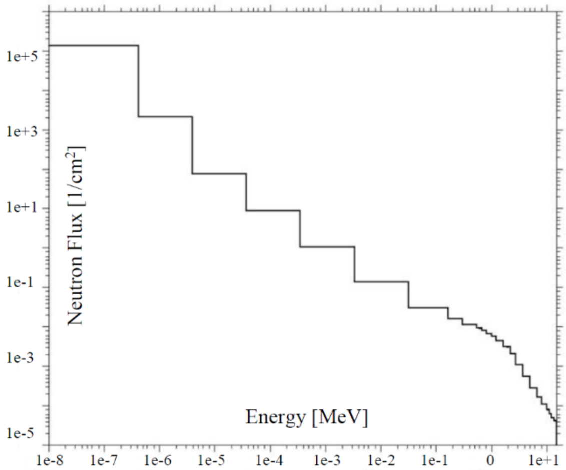

Figure 2: Neutron Flux Distribution by Energy

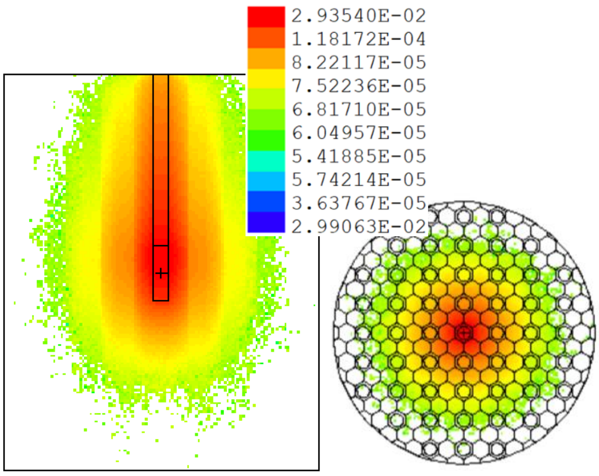

Figure 3: Neutron Flux Distribution in Core

As a result of this simulation energy distribution of neutrons were obtained alongside with neutron flux values, which can futher serve for reaction rates determination. Neutron flux in the case of loaded core is shown in figure 3. It is important to note here that the values presented in figure are those that corresponds to one source particle interaction.

2) ASSESMENT OF $keff$

A set of simulations were carried out for investigation of several salts behavior in molten medium with a nuclear $Th - U$ fuel. Every simulation carried out with fixed 80% nuclear fuel but different salt composition. As a result of simulations k_{eff} multiplication values were obtained with corresponding errors, which are shown in Table. 2.

$\boldsymbol{ThU}$ - Salt Composition	$\boldsymbol{keff}$	Error
LiCl	0.33819	0.00017
LiCl-KCl	0.37304	0.0002
LiF-KF	0.92074	0.00045
LiF-ZrF_4	0.95588	0.00045
LiF-NaF-KF	0.92332	0.00042
LiF-NaF-RbF	0.93949	0.00046
LiF-BeF_2-ZrF_4	0.95366	0.00044
LiF-RbF	0.94077	0.00043
LiF-BeF_2	0.95394	0.00043
LiF-CaF_2	0.95123	0.00058
KNO_3	0.87783	0.00044
$NaNO_3$	0.89782	0.00042
NaCl-KCl	0.42101	0.00022
KCl	0.44416	0.00022

Table 2: Chemical Compositions of Molten Salts

According to the table, the lowest k_{eff} was calculated for chlorides compositions and the biggest for alkali and alkaline metal fluorides. Especially bigger ones are those containing beryllium and/or zirconium. Relatively big criticality values were obtained for nitrides, however not much to be used in proposed reactor design. Alkali and alkaline metal salts compositions showed appropriate results for the Accelerator Driven Molten Salt Reactor operation, as according to its design the lack of 5-10% should be covered by external accelerator source.

Neutron flux with relatively high k_{eff}value, in particular, LiF – ZrF_4 salt is shown in Figure 4 distributed by several energy bins. For comparison with flux obtained for salt, which showed low multiplication factor, neutron flux of LiCl – CaCl presented in Figure 5. According to the graphs, difference in neutron flux between these cases are negligible, hence different k_{eff}values are conditioned mostly by absorption cross section differences of salt additions.

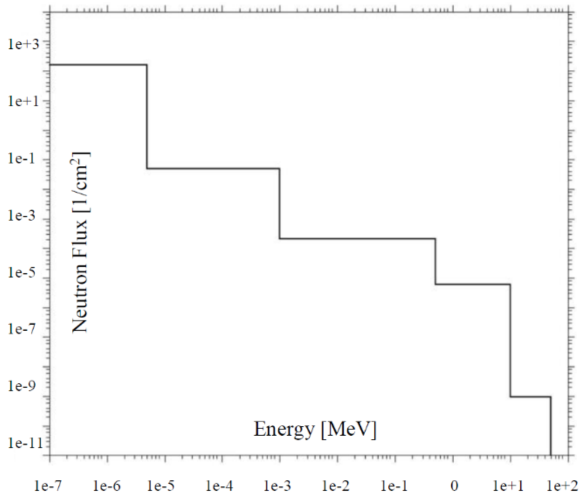

Figure 4: Neutron Flux LiF-ZrF4

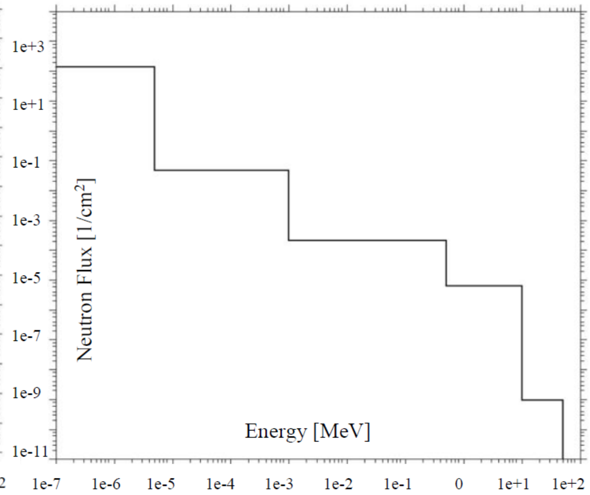

Figure 5: Neutron Flux LiCl-CaCl

4 CONCLUSION

In the current study, the model of conceptual Molten Salt Reactor was developed for MCNP analysis. A set of simulations were carried out for investigation of behavior of lead target under 800MeV proton beam, by getting the results for neutron flux, energy distribution, as well as criticality assessment for several types of salts as a part of medium of nuclear fuel. Neutron fluxes and energy distribution visualization are shown as a part of the current work. The results of neutron fluxes can be further served for determination of reaction rates in the core of proposed reactor. Around 16.14 neutrons were found to be produced per incident proton, which is 3-4 neutrons less than current MSR reactor purposes. According to $\boldsymbol{k_{eff}}$assessments, alkali metal fluoride salts showed appropriate value to be considered alongside $Th-U$ fuel cycle, being slightly lower from critical value to be balanced by accelerator.

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