The Effect of Nuclear Data Discrepancies on Criticality Simulations of Molten Salt Fast Reactors

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INTRODUCTION

The Molten Salt Fast Reactor (MSFR) is a fast spectrum MSR, part of the generation IV reactor concepts, and has a unique design utilizing fuel in the form of molten salt mixture. A combination of fissile material dissolved in molten liquid salt creating unique characteristics of the fuel such as it acts as the carrier of the fissile elements and the coolant to the system. The combinations of the molten salt, the fuel breeding ability, and the closed fuel cycle creates a very efficient and safe reactor that addresses the concern of nuclear waste and material sourcing [1].

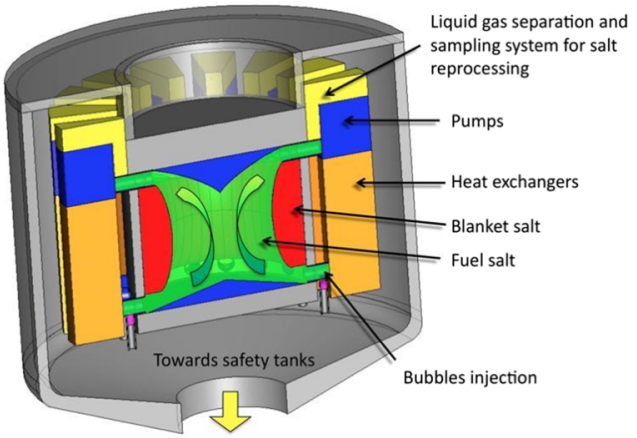


Fig. 1. Schematic MSFR design from the EVOL project [1].

The reactor has been studied throughout many countries, including Russia, the United States and European countries. A commonly accepted MSFR design concept amongst these countries is shown in Fig. 1. This paper will focus on main design components of the common concept, including the fuel salt, the fertile salt, shielding, and reflectors. Amongst them, fertile salt commonly utilizes thorium as its fertile element, shielding/protection (neutron shielding) composed of , and reflectors are normally made by a Ni-based alloy.

The fuel material composition, however, currently still has much speculation amongst different MSFR design projects. Three common fissile materials are accepted and used in most MSFRs designs: ^{233}U, transuranic elements (TRU), or a mixture of enriched uranium in combination with transuranic elements (TRU/U^{enr}) [1]. For the molten salt base there are two different elements that have been considered. In combination with these fissile elements the molten salt that has been most studied is fluoride molten salt. Several research projects such as the Molten Salt Research Experiment (MSRE) at Oakridge National Laboratory [2] and in the EVOL/MARS [1] collaborative project in Russia have studied fluoride molten salt in MSRs and MSFRs for several years. New research groups and companies have been exploring an alternative fuel type using chloride molten salt which is studied much less than fluoride. One such company is TerraPower who have been investigating and working towards creating an operational Molten Chloride Fast Reactor (MCFR) [3].

As the MSFR is a highly theoretical model it is entirely based on neutronics calculations, modeling, and simulation so ensuring the precision of these calculations is vital for these reactors to work as expected once in operation. The work of this paper will focus on a factor that can impact such results: nuclear data libraries. In neutronics simulations nuclear data libraries are the foundation of information that these neutron transport codes run on. A reactor model geometry and composition can be identical, but a difference in nuclear data library being used as input can alter the reactor calculations. This work will investigate discrepancies in such libraries and their impact on neutronics calculations using MSFR design.

In this work the reference design of the MSFR provided in Ref. [1] is used as the base reactor model for studying the sensitivity of the reactor criticality (k_{eff}) and other representative reaction rates to the cross-section libraries. A TRU/U^{enr} fuel mixture in a chloride-based nolten salt provided in Ref. [4] will be studied. The sensitivity of the reactor criticality will be compared using the two newest libraries of the Evaluated Nuclear Data Files (ENDF) [5].

NUCLEAR DATA DISCREPANCIES

The National data nuclear center (NNDC) is website that houses the nuclear data libraries that are used across different research areas. These include libraries such as different versions of the ENDF, Joint Evaluation Fission and Fusion Library (JEFF), and Japanese Evaluated Nuclear data (JENDL), and so on [5]. This paper will focus on libraries in ENDF/B-VIII.0 and ENDF/B-VII.1, as these versions are

more recently published and most used in the United States research projects.

The data that makes up each of these libraries are produced and compiled by nuclear physics researchers. Every couple of years a new library version will be published with new results and measurements. The nuclear data reported for certain isotopes depends solely on what is reported and what is a highly studied isotope in the field of nuclear physics. Three isotopes with lots of reported data are ^{233}U, ^{235}U, and ^{238}U. These isotopes of uranium are the fissile and fissionable material in the three fuel compositions being considered and therefore play a large role in the criticality calculation of the reactor.

To investigate the potential of difference in library versions and the magnitude of such difference, the energy-dependent total neutron cross section can be graphed. On pointwise graphs such discrepancies are hard to visualize but a discrete difference can be seen when graphed in a groupwise format. The open-source code NJOY2016 processes ENDF files under different conditions to prepare them as ACE files to be read by Monte Carlo based reactor simulation codes such as MCNP, Serpent, and OpenMC. One of the processes that NJOY is capable of is GROUPR, a module of the code that calculates averages of pointwise cross sections and multigroup matrices, which describes the transfer of neutrons from one group to the next [6]. On a graph, this allows for the total cross sections of data to be broken down into a groupwise format. Such a format produces a visual that shows distinct differences in the libraries, mostly seen in the resonance region. Fig. 2 shows a comparison of the group-wise total neutron cross section of ^{235}U provided by ENDF/B-VIII.0 and ENDF/B-VII.1, respectively. It is important to note that the plot is log-scaled and hence the differences in the cross section are significant.

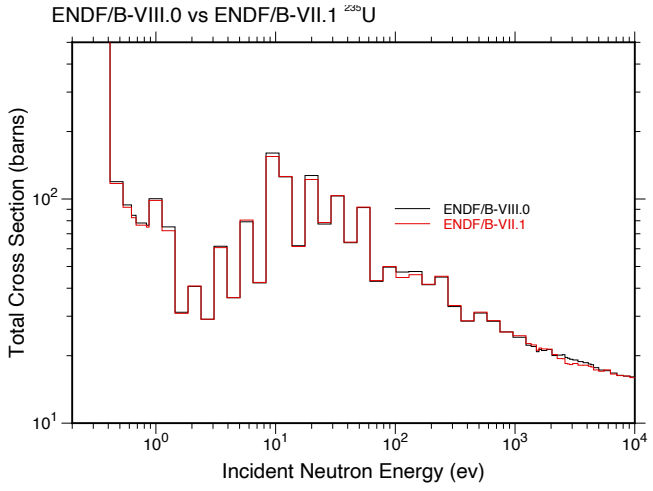
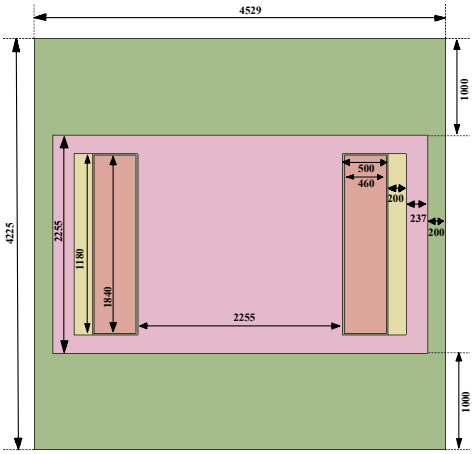


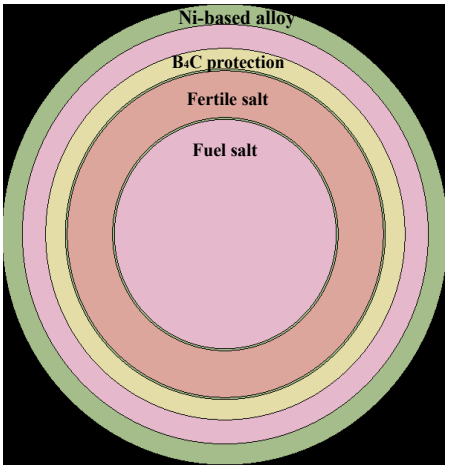
Fig. 2. Comparison of ENDF/B-VIII.0 and ENDF/B-VII.1 nuclear data libraries for 239 group total cross section of ^{235}U zoomed on the resonance range.

NUCLEAR REACTOR MODEL

Serpent is used for modeling the MSFR in this work. Serpent a Monte Carlo based neutron transport code capable of performing reactor physics calculations such as criticality analysis, burn up, radiation shielding, etc. One of the primary applications of the Serpent code is to model and simulate nuclear reactors [7]. The geometry of the MSFR is shown in Fig. 3. The geometry has four parts: the fuel salt (light pink), the fertile salt (orange), the B_4C protection (yellow), and the walls/reflectors (green). The geometry is subject to vacuum boundary condition. The molar compositions of all materials are provided in Table I, Table II, and Table III. The B_4C with a density of 2.52 g/cm^3 is the protection on the exterior of the fertile blanket and acts as the neutron shielding and protection for the heat exchangers. The Ni-based alloy walls act as neutron reflectors with a density of 10 g/cm^3. All materials, including the fuel, are assumed with the temperature of 973K in all the calculations [3].



(A)



(B)

Fig. 3. Axial planar view (A) and radial planar view (B) of the MSFR core model (dimensions given in mm).

The fuel salt as mentioned before can take varying compositions depending on the choice of molten salt and fertile elements. For the current study, a fuel mixture of enriched uranium and TRU from typical spent UOX fuel in a chloride based molten salt is studied [4]. Chloride is enriched to 99.99% in ^{37}Cl.

Table I. Molar Composition and density of molten salts.

Material	Molar Composition	Density [g/cm^3]
TRU/ U^{enr} -Chloride	NaCl (50%) $ThCl_4$ (20.8%) U^{enr} Cl_3 (21%) $TRUCl_3$(8.2%)	3.26
Fertile salt	NaCl (70%) $ThCl_4$ (30%)	2.65

Table II. Molar Composition and density of core materials.

Material	Molar Composition	Density [g/cm^3]
Shield	B (80%), C (20%)	2.52
Reflector	Ni (79.432%), W (9.976%), Cr (8.04%), Mo (0.736%), Fe (0.632%), Ti (0.295%), C (0.294%), Mn (0.257%), Si (0.252%), Al (0.052%), B (0.033%), P (0.023%), S (0.004%)	10.0

The simplified MSFR model is developed using Serpent and the model is used to calculate the k_{eff} value of the reactor. The reported compositions correspond to the critical composition [4]. It's important to note that critical composition was calculated based on the ENDF/B-VII.0 and JEFF-3.1 material libraries. Thus, a deviation in k_{eff} is expected due to the use of different material libraries in this work .

Table III. Composition of TRU elements from spent UOX fuel.

Material	Mole Composition
TRU	^{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 (1.8%)
	^{245}Cm (0.1%)

RESULTS AND DISCUSSION

The results of the eigenvalue simulation for the two materials libraries are summarized in Table IV. The deviation in the k_{eff} calculated using the two cross section libraries is about 4000 pcm. This large deviation in the k_{eff} indicates that the neutronics simulation is sensitive to the utilized material library. To further investigate the difference between the two libraries, the integral reaction rates as estimated by the two libraries are compared in Table V. The results show that ENDF/B-VII.1 underestimates the fission rate by about 4% and the leakage rate by about 23% compared to ENDF/B-VIII.0.

Table IV. TRU/U^{enr}-Chloride fuel k_{eff} Results.

ENDF/B-VII.1	ENDF/B-VIII.0	Absolute Difference in[pcm]
0.974182 ±0.00007	1.01372 ±0.00007	-3953.8

Table V. TRU/U^{enr}-Chloride fuel reaction rate comparison.

Integral Reaction Rate	ENDF/B-VII.1	ENDF/B-VIII.0	Relative % difference
Fission	0.34468	0.358892	-4.12
Absorption	0.998896	0.998558	0.03
Capture	0.654216	0.639667	2.22
Leakage	0.001103	0.001440	-23.37

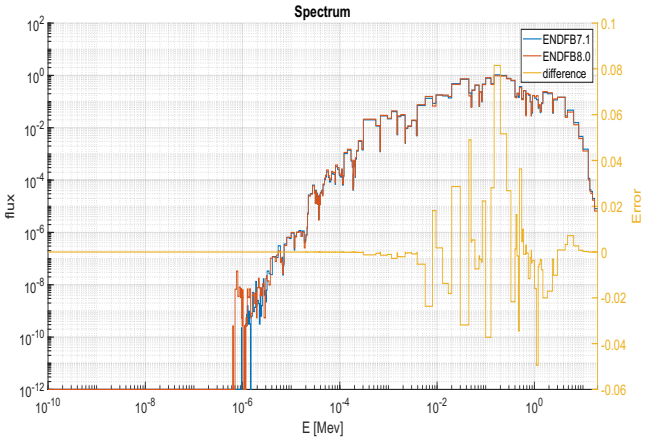


Fig. 4. Neutron energy spectrum of ENDF/B-VII.1 vs. ENDF/B-VIII.0.

The difference in the normalized group-wise neutron spectrum as predicted by the two libraries are shown in Fig. 4. The results show that there is a non-negligible difference in the group-wise spectrum.

CONCLUSIONS AND FUTURE WORK

Using the MSFR research reactor from the EVOL project as a template, this work investigated reactor criticality sensitivity to cross section libraries. The reactor model utilized also the newly proposed chloride molten salt base with spent UOX fuel from LWRs. The newest ENDF nuclear data libraries ENDF/B-VII.1 and ENDF/B-VIII.0 were used to simulate and compare the criticality results and reaction rates of the three fluoride and three chloride molten salt fuels using Serpent version 2.2.1.

The results showed a difference as large as 4000 pcm in k_{eff} values can result when modeled with both the ENDF/B-VII.1 and ENDF/B-VIII.0 libraries. This shows that neutronics calculations are sensitive to nuclear data library inputs. Considering the sensitivity of neutronics calculations to cross section data, it is expected that newer libraries with more reported data can produce more accurately simulated reactors. To further understand the extent of nuclear data cross sections' effect on reactor performance, other reactor parameters were investigated including integral reaction rates and neutron spectra. The results showed non-negligible differences in the predicted reaction rates up to 23% for the neutron leakage rate. Also, the group-wise neutron spectrum shows dependance on the nuclear data library.

Future work will investigate other parameters such as flux distributions, DNPs parameters, and reactivity feedback coefficients. Moreover, a more detailed analysis of the energy and isotopic dependance of different reaction rates will be considered to reveal the underlying sources of discrepancy between the two libraries. Another interesting area of research is model verification using OpenMC and MCNP to rule out the neutron transport codes as a source of difference in reactor calculations.

Considering that nuclear data has showed to influence neutronics calculations, moving forward it is important for researchers to model with the most up to date data libraries. A data library with more data will produce the most accurate calculations. Therefore, rather than focusing on comparing older and newer versions of the same libraires, future work should consider the difference in neutronics calculations from newest versions of nuclear data libraries that are utilized in different countries such as JEFF, JENDL, and ENDF. Such comparative studies will help researchers to know which nuclear data libraries are best for calculations, even if they aren't the most accepted libraries in their given country.

ACKNOWLEDGMENTS

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