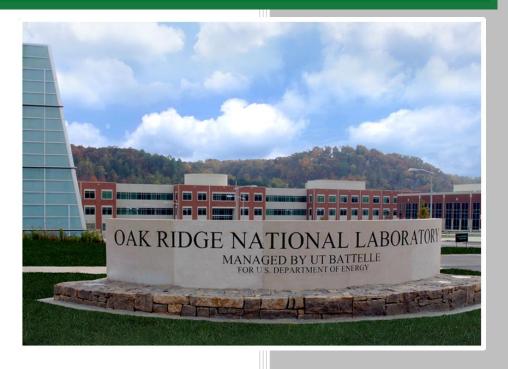
Complete Sensitivity/Uncertainty Analysis of LR-0 Reactor Experiments with MSRE FLiBe Salt and Perform Comparison with Molten Salt Cooled and Molten Salt Fueled Reactor Models



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Nicholas R. Brown Jeffrey J. Powers Donald E. Mueller Bruce W. Patton

December 2016

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Reactor and Nuclear Systems Division

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Date Published: December 31, 2016

Prepared by
OAK RIDGE NATIONAL LABORATORY
Oak Ridge, TN 37831-6283
managed by
UT-BATTELLE, LLC
for the
US DEPARTMENT OF ENERGY
under contract DE-AC05-00OR22725

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ACRONYMS AND ABBREVIATIONS

AHTR Advanced High Temperature Reactor

DOE US Department of Energy

FHR fluoride salt-cooled high temperature reactor

FLiBe 2 ⁷LiF-BeF₂ salt FY fiscal year

IRPhE International Reactor Physics Experiment Evaluation

LEU low-enriched uranium MSR molten salt reactor

MSBR Molten Salt Breeder Reactor MSRE Molten Salt Reactor Experiment

NE Office of Nuclear Energy

ORNL Oak Ridge National Laboratory

RC Řež Research Centre Řež S/U sensitivity and uncertainty

ACKNOWLEDGMENTS

This work was supported by the US Department of Energy's Office of Nuclear Energy (DOE-NE) Advanced Reactor Technologies program. The authors would like to recognize the outstanding collaboration of Michal Košťál, Evžen Losa, Jan Uhlíř, Miroslav Hrehor, Ján Milčák, and the other researchers at Research Centre Řež in the Czech Republic. Their efforts and hospitality are greatly appreciated.

The Advanced High Temperature Reactor (AHTR) model used for sensitivity/uncertainty analysis in this report is based on a model used as part of the AHTR design studies by Dan Ilas. The Molten Salt Breeder Reactor model used for sensitivity/uncertainty analysis in this report is based on a model developed in support of the Fuel Cycle Options Campaign by Jeffrey Powers, Ben Betzler, Thomas J. Harrison, and others.

Important contributions and feedback on S/U analysis provided by William J. Marshall are gratefully acknowledged, including guidance on how specific issues related to code input and output. Suggestions and guidance from Matt Jessee and Christopher Perfetti on the underlying S/U methods in SCALE and specifics of code input files were also helpful.

The authors also thank David Holcomb, the DOE-NE Advanced Reactor Technologies Technical Area Lead for salt reactors, for his review and insights. Helpful review comments were provided on this report by Ben Betzler, Thomas J. Harrison, and Rose Raney.

EXECUTIVE SUMMARY

In September 2016, reactor physics measurements were conducted at Research Centre Řež (RC Řež) using the FLiBe (2 ⁷LiF + BeF₂) salt from the Molten Salt Reactor Experiment (MSRE) in the LR-0 low power nuclear reactor. These experiments were intended to inform on neutron spectral effects and nuclear data uncertainties for advanced reactor systems using FLiBe salt in a thermal neutron energy spectrum.

Oak Ridge National Laboratory (ORNL), in collaboration with RC Řež, performed sensitivity/uncertainty (S/U) analyses of these experiments as part of the ongoing collaboration between the United States and the Czech Republic on civilian nuclear energy research and development. The objectives of these analyses were (1) to identify potential sources of bias in fluoride salt-cooled and salt-fueled reactor simulations resulting from cross section uncertainties, and (2) to produce the sensitivity of neutron multiplication to cross section data on an energy-dependent basis for specific nuclides.

This report provides a final report on the S/U analyses of critical experiments at the LR-0 Reactor relevant to fluoride salt-cooled high temperature reactor (FHR) and liquid-fueled molten salt reactor (MSR) concepts. In the future, these S/U analyses could be used to inform the design of additional FLiBe-based experiments using the salt from MSRE.

The key finding of this work is that, for both solid and liquid fueled fluoride salt reactors, radiative capture in ⁷Li is the most significant contributor to potential bias in neutronics calculations within the FLiBe salt.

This milestone (M3AT-17OR2401091) is a revised, expanded version of a preliminary status report issued in August 2016 (M4AT-16-OR2401094). As part of the present work package, ORNL accomplished the following in support of the international collaboration with RC Řež:

- In May 2016 and September 2016, delegations from the United States visited the Czech Republic. The May 2016 visit included observations of experimental operations at the LR-0 reactor, as well as collaborative discussions on how S/U analysis can enhance experiments in LR-0. The September 2016 visit focused on FLiBe experiments and discussion of the study's preliminary findings.
- A three-dimensional model of the LR-0 reactor was developed using the SCALE code system.
 The detailed model shows excellent agreement with draft benchmark evaluations intended for the International Handbook of Evaluated Reactor Physics Benchmark Experiments.
- Scoping S/U analyses were performed for several example configurations of the LR-0. Due to higher sensitivity to nuclear data with higher uncertainty, key sources of potential bias for a baseline configuration (without any insertions in the central experimental zone) of the LR-0 include the average number of neutrons released per ²³⁵U fission and neutron scattering in ²³⁸U.
- Application models were adapted for S/U analysis of FHR and MSR concepts. These models are representative of the Advanced High Temperature Reactor (AHTR) and Molten Salt Breeder Reactor (MSBR) designs. One challenge beyond the scope of this work is that the application models are at or above 700 °C, but the neutron cross section covariance data libraries are for room temperature.

- The models were used to perform initial scoping S/U analyses for FHR and MSR concepts. An objective of the LR-0 experiments should be to generate experimental configurations that reproduce key sensitivities. The most significant potential source of bias within the FLiBe salt in configurations cooled or fueled by FLiBe is radiative capture in ⁷Li.
- Differences in the energy dependence of the key FLiBe sensitivity coefficients in the LR-0 and in the advanced reactor application models were identified. These differences primarily arise due to the different neutron energy spectral characteristics related to neutron moderation in water versus graphite.

Several important areas of possible future work were also identified:

- S/U analysis should be conducted on prior experiments, including those with FLiNa salt, to determine the potential relevance to the FHR application models.
- All FHR and MSR S/U analyses in this work modeled fresh fuel without fission products, thus approximating beginning of life conditions for reactor concepts. Analysis of middle of life and end of life fuel compositions with corresponding fission product inventories should be performed in the future, though no directly relevant experiments yet exist to provide validation data for these analyses.
- Experiment designs should be pursued that could enable LR-0 experiments to gather data relevant to reactivity coefficients in FHRs and MSRs. Examples include temperature-dependent reactivity worth of salt and assessing void reactivity worth in salt.

1. INTRODUCTION

There is an ongoing collaboration between the United States and the Czech Republic on civilian nuclear energy research [1, 2]. Recent activity includes a joint declaration in 2010 between the US Department of Energy (DOE) and the Department of Commerce and the Ministry of Industry and Trade of the Czech Republic [1]. In addition, a Memorandum of Understanding on Cooperation in Nuclear Energy between DOE and the Czech Ministry of Industry and Trade was signed in Prague on December 12, 2012. This collaboration has included the delivery of 75 kg of FLiBe (2 ⁷LiF + BeF₂) fluoride salt from the Molten Salt Reactor Experiment (MSRE) at Oak Ridge National Laboratory (ORNL) to the Research Centre Řež (RC Řež) [1,3]. More recently, an Agreement for Cooperation in Civilian Nuclear Energy Research and Development was executed in 2014 [2].

The collaboration on MSRE salt was extended in fiscal year (FY) 2016 and the first quarter of FY 2017 with the DOE Office of Nuclear Energy (NE) Advanced Reactor Technologies project. The effort is aimed at sensitivity/uncertainty (S/U) analyses of reactor physics experiments with FLiBe salt to be performed in the LR-0 low power reactor [4,5]. These experiments are intended to be a benchmarking data source to validate neutronics calculations for liquid fueled molten salt reactor (MSR) and fluoride high-temperature salt-cooled reactor (FHR) concepts [1]. MSRs are a class of advanced nuclear reactor that uses liquid fluoride or chloride salts either as a coolant with a solid fuel (as in FHRs) or with a fuel dissolved in liquid salt that also serves as the coolant material. This milestone (M3AT-17OR2401091) is a revised, expanded version of a preliminary status report issued in August 2016 (M4AT-16-OR2401094) [6]. It is a final report intended to document several specific ORNL team technical accomplishments that directly support the collaboration with RC Řež.

The S/U analyses in this project are useful to assess the LR-0 experiments using US-origin FLiBe salt provided to the Czech Republic in 2012. The present collaboration is focused on measuring the reactor physics impacts of FLiBe salt enriched in ⁷Li. The objective of the present effort is to have high-quality critical experiments to validate reactor physics calculations for fluoride salt reactor concepts. These critical experiments should be useful for reactor operations and reactor design. An additional objective is to assess the adequacy of ENDF/B-VII.1 cross sections for analysis of fluoride salt reactor concepts.

S/U analysis identifies potential sources of bias due to neutron cross sections through uncertainty analysis. The sensitivity to a specific reaction in an energy regime of interest is used to assess the efficacy of an experiment relative to the particular sensitivity. The sensitivity profiles as a function of energy can be applied as a tool to design informed experiments to address those potential sources of bias. A general schematic of the overall approach to S/U analysis as part of this collaboration is shown in Figure 1.

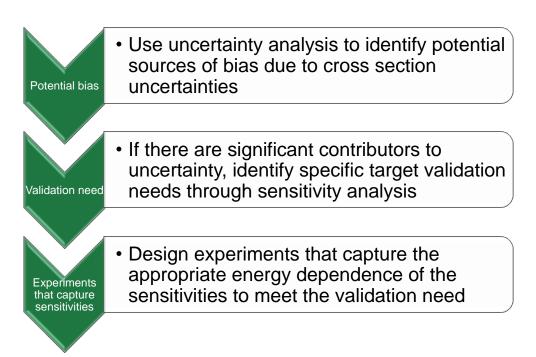


Figure 1. S/U analysis approach to enhance MSRE FLiBe experiments.

The S/U evaluation performed in this project assessed whether the desired neutron parameter sensitivities are achieved with the conducted experiments (e.g., neutron cross section sensitivity for specific isotopes). In addition, the S/U analyses were used to identify potential nuclear data deficiencies with regard to FHR and MSR designs and quantify target nuclear data improvements needed to support modeling and simulations needs. As part of possible future work, the S/U analysis approach in this report can be used to support development of a benchmark evaluation for the proposed LR-0 critical experiments and develop a roadmap of data needs and recommendations for future experiments and collaborations. The approach can also be used to evaluate previous experiments with FLiNa salt to better examine their relevance to systems using FLiBe or other salts.

In support of the collaboration, ORNL research staff travelled to the Czech Republic in May 2016 to develop a better understanding of the LR-0 reactor and its capabilities and to discuss past and proposed experiments with facility staff. In September 2016, ORNL staff returned to the Czech Republic to obtain an update on the experiments and discuss the S/U analysis approach and initial results.

The ORNL effort focused on S/U analysis of the LR-0 FLiBe experiments using ORNL tools, including TSUNAMI-3D [7] from the SCALE code system [8] using continuous energy (CE) cross sections. This S/U information may enable development of more impactful experiments at the LR-0 and can improve the usefulness of the reactor physics experiments conducted using the FLiBe salt.

Simplified two-dimensional (2D) and detailed three-dimensional (3D) models of the LR-0 reactor were developed using the SCALE code system. The detailed 3D models show excellent agreement with reference draft benchmarks intended for the benchmark handbook of the International Reactor Physics Experiment Evaluation (IRPhE) Project [9] and references in the open literature [10,11].

Scoping S/U analyses were performed for several example configurations of the LR-0. In addition, application models were adapted for S/U analysis of FHR and MSR concepts. These models are

representative of the Advanced High Temperature Reactor (AHTR) [12] and Molten Salt Breeder Reactor (MSBR) [13] designs. The application models were used to perform initial scoping S/U analyses for FHR and MSR concepts. The objective of the LR-0 experiments performed by RC Řež was to investigate the adequacy of nuclear data for FLiBe constituents by comparing computational models against integral reactivity experiments and possibly generate new IRPhE benchmark entries. The ORNL S/U analysis of the LR-0 FLiBe experiments assessed the ability of the experimental configurations used, as well as other possible configurations, to reproduce these sensitivities for nuclides that are significant potential sources of bias due to neutron cross sections. Although it is outside the scope of the present work, the fact that the application models are at or above 700 °C but the neutron cross section covariance data are at room temperature should be considered in future work.

Each of these technical outcomes directly advances the objectives of this project. One objective is to evaluate the suitability of experiments performed at the LR-0 reactor in the Czech Republic for use as validation data for MSR design and operation. Another objective is to use knowledge gained from evaluating the LR-0 reactor experiments to generate recommendations for future experiments, which are expected to involve US-origin isotopically selected FLiBe salt obtained from ORNL's MSRE, thereby ensuring that the desired neutron parameter sensitivities are achieved with the proposed experiments (temperature coefficient of reactivity, neutron cross section sensitivity for specific isotopes, etc.). It is expected that this S/U analysis will help assess the adequacy of US nuclear data (i.e., ENDF/B) applied to MSR systems and generate recommendations for data improvements.

This milestone report includes development of models of LR-0 with SCALE, S/U analysis of LR-0 configurations, S/U analysis of application models, and plans for future work. In addition, the appendices include summaries of the May 2016 and September 2016 ORNL visits to RC Řež.

2. ORNL MODELING OF LR-0 REACTOR AND SENSITIVITY/UNCERTAINTY ANALYSIS OF A TYPICAL LR-0 CONFIGURATION

This section provides a brief overview of ORNL activities modeling the LR-0 reactor.

2.1 OVERVIEW OF THE LR-0 REACTOR

The LR-0 reactor is a low power reactor (critical assembly) pool type research reactor at RC Řež using partial height (1/3rd) VVER assemblies. These assemblies are radially identical, but with a reduced height relative to a VVER-1000 fuel assembly. The continuous maximal operating power is on the order of 1 kW, and the thermal neutron flux density is 10⁹ n/(cm²-sec) [10]. The LR-0 reactor must have at least six fuel assemblies in a critical configuration, but it can have significantly more. For example, the VVER mini-core mockup has thirty-two ½-height assemblies of three different uranium enrichments [5]. Reactor criticality is controlled using the height of the water moderator, and there are a variety of instrumentation tubes and possible configurations. A photograph from the top of LR-0 during refueling is shown in Figure 2, and the features of the LR-0, including a detailed diagram of the reactor, are shown in Figure 3.



Figure 2. LR-0 reactor photograph during refueling with top cover removed, with five fuel assemblies in the core and the water moderator drained.

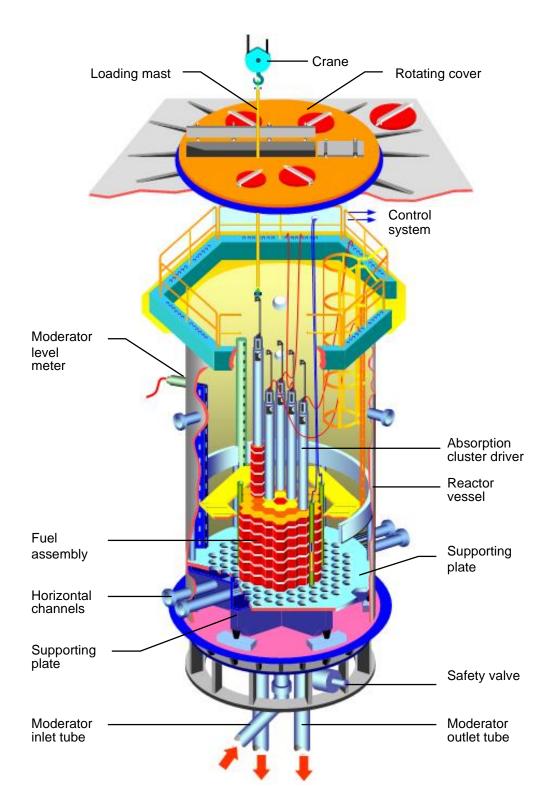


Figure 3. LR-0 reactor diagram [9].

2.2 LR-0 REACTOR MODELING

A detailed 3D SCALE [8] model of the LR-0 reactor was developed and used to analyze two example systems from Reference 11. The key features of the LR-0 reactor were included, including the fuel assemblies, the water moderator height, the lower support plate, and the un-moderated upper portion of the core. For the SCALE model, the lower plate and grid spacers were homogenized. A KENO 3D isometric projection view of the model is shown in Figure 4.

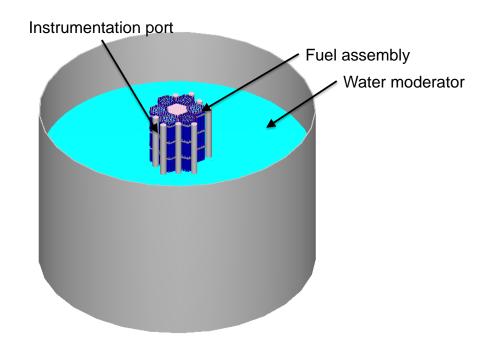


Figure 4. KENO3D isometric projection view of the LR-0 SCALE model.

An axial slice view of the model is shown in Figure 5, and a planar slice view of the fuel assemblies is shown in Figure 6.

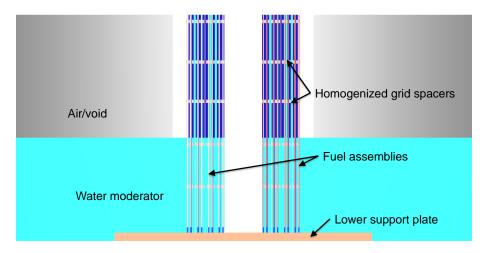


Figure 5. Axial slice view of the LR-0 SCALE model.

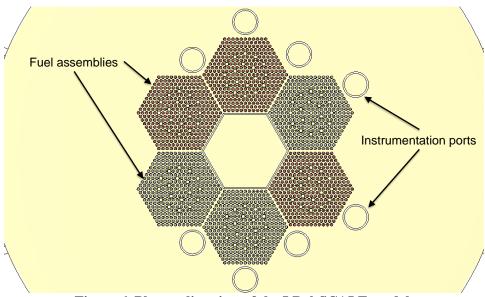


Figure 6. Planar slice view of the LR-0 SCALE model.

The model was used to generate eigenvalue and S/U analysis results for two cases presented in References 9 and 11. The first case, referred to as Case 1 in Reference 9, consists of a baseline LR-0 configuration with six fuel assemblies of approximately 3.3% enrichment. The second case, referred to as Case 16 in Reference 9, is identical to the first case, but it includes an inserted zone of natural FLiBe (e.g., no enrichment in ⁷Li) in an Inconel container. A comparison between the measured critical moderator height in centimeters and the calculated neutron multiplication factor calculated using the KENO-VI sequence at the specified moderator height is shown in Table 1. With the exception of the data in Table 1, all other results in this report used ENDF/B-VII.1 libraries with CE cross sections. The calculated effective multiplication factor is close to unity in all cases, indicating that the model of the LR-0 reactor is reasonable.

Table 1. Effective multiplication factor for two example LR-0 configurations calculated with KENO using the ENDF/B-VII.0 and ENDF/B-VII.1 nuclear data libraries

Configuration	Measured critical Calculated $k_{\it eff}$		ated $k_{\it eff}$
	moderator height (cm)	ENDF/B-VII.0,CE	ENDF/B-VII.1,CE
Case 1 (base case)	55.639	1.00633 ± 0.00023	1.00524 ± 0.00023
Case 16 (Natural FLiBe)	57.736	1.00497 ± 0.00022	1.00448 ± 0.00025

Using the TSUNAMI-3D sequence, the potential sources of bias due to cross section data in the LR-0 reactor were identified. These key uncertainties are similar to other light water reactors [7] and are shown in Table 2. Negative uncertainties in eigenvalue are due to anti-correlated covariance data, or shared uncertainty for two closely related quantities.

Table 2. Top contributors to uncertainty in effective multiplication factor from cross section covariance data for the LR-0 reactor using ENDF/B-VII.1 CE cross sections

Nuclide	Reaction	Covariance w/nuclide	Reaction	Uncertainty in $k_{\it eff}$ (%delta-k/k)
Total	N/A	N/A	N/A	6.40E-01 ± 2.3E-04
^{235}U	nubar	^{235}U	nubar	$3.54E-01 \pm 5.62E-05$
^{238}U	n,n'	^{238}U	n,n'	$3.02\text{E-}01 \pm 1.36\text{E-}03$
^{238}U	n,gamma	^{238}U	n,gamma	$2.40E-01 \pm 1.92E-05$
^{235}U	chi	^{235}U	chi	$2.39E-01 \pm 1.44E-03$
^{238}U	n,n'	^{238}U	elastic	-1.79E-01 ± 1.21E-03
^{235}U	n,gamma	^{235}U	n,gamma	$1.66\text{E-}01 \pm 9.51\text{E-}06$
^{235}U	fission	235 U	n,gamma	$1.18E-01 \pm 1.09E-05$
^{1}H	n,gamma	$^{1}\mathrm{H}$	n,gamma	$1.11E-01 \pm 4.03E-06$
^{235}U	fission	^{235}U	fission	$1.06\text{E-}01 \pm 1.68\text{E-}05$
1 H	elastic	$^{1}\mathrm{H}$	elastic	$1.06E-01 \pm 3.56E-05$
^{16}O	elastic	¹⁶ O	elastic	$1.01\text{E-}01 \pm 1.56\text{E-}04$
⁵⁶ Fe	n,gamma	⁵⁶ Fe	n,gamma	$9.17E-02 \pm 5.54E-06$
^{238}U	nubar	^{238}U	nubar	$6.21E-02 \pm 1.23E-05$
^{238}U	elastic	^{238}U	elastic	$5.70E-02 \pm 2.04E-04$
91 Zr	n,gamma	91 Zr	n,gamma	$4.19E-02 \pm 1.12E-06$

In sensitivity and uncertainty analysis, the eigenvalue sensitivity coefficient is defined as

$$S_{k,\Sigma} = \frac{\delta k/k}{\delta \Sigma/\Sigma}$$
,

where Σ is the system parameter (e.g., cross section) with a given uncertainty. The energy dependence of the eigenvalue sensitivity coefficients for the 3D model and the 2D scoping model were also considered. In general, the energy dependence and shape of the sensitivities as a function of energy were very similar for the two cases. Examples from top contributors shown in Table 2 include ²³⁵U nubar in Figure 7, ²³⁸U radiative capture in Figure 8, and ¹H elastic neutron scattering in Figure 9. The total sensitivity values in the LR-0 model were verified using direct perturbation of the moderator density, resulting in nearly identical total sensitivities for the direct perturbation and the TSUNAMI-3D calculation.

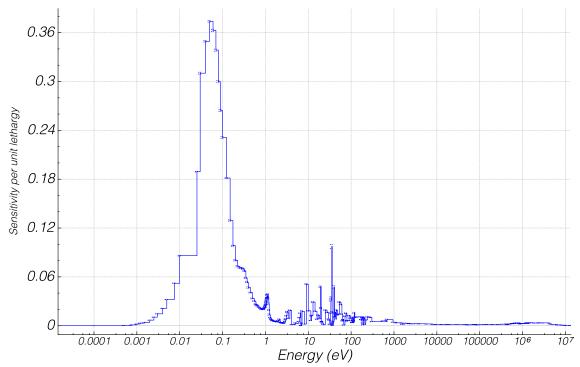


Figure 7. ²³⁵U nubar sensitivity coefficients for the 3D LR-0 model without FLiBe salt.

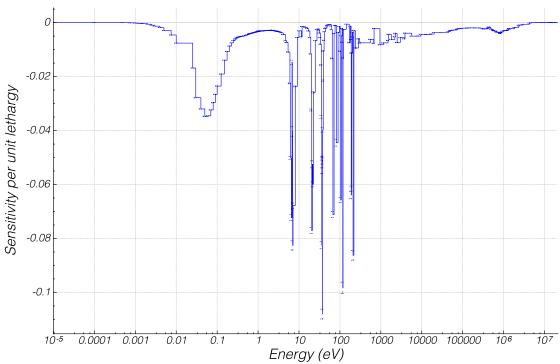


Figure 8. ²³⁸U (n, gamma) sensitivity coefficients for the 3D LR-0 model without FLiBe salt.

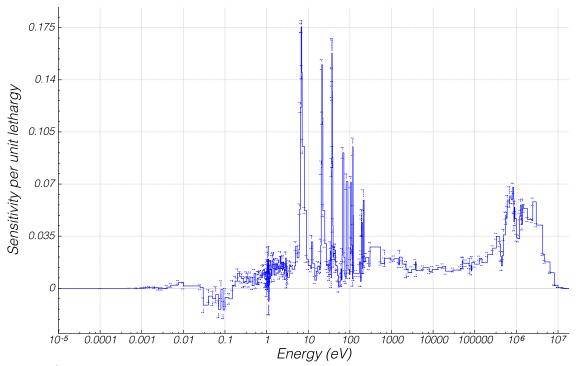


Figure 9. ¹H elastic scattering sensitivity coefficients for the 3D LR-0 model without FLiBe salt.

2.3 PRELIMINARY S/U ANALYSIS OF SEPTEMBER 2016 LR-0 EXPERIMENTS WITH MSRE FLIBE

In September 2016, RC Řež performed critical experiments in LR-0 with MSRE FLiBe. Prior experiments focused on FLiBe salt with natural lithium [11], with a few limited experiments performed using a small amount of MSRE salt [1]. One key aspect of the September experiments is that the MSRE salt consists of approximately 99.99+% ⁷Li [14], which is representative of an operational MSR or FHR. However, the exact ⁷Li enrichment of the MSRE salt used in the experiment is currently unknown; efforts to determine this parameter may occur at RC Řež in the near future. RC Řež provided engineering drawings of the FLiBe insertion zone for the September 2016 experiments. An example planar view of the insertion zone is shown in Figure 10, indicating dimensions and radial features of the design.

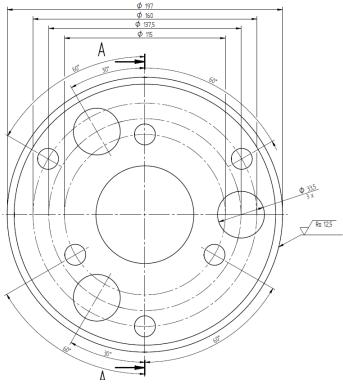


Figure 10. Planar view of the new FLiBe inserted zone for September 2016 experiments in the LR-0 Reactor (drawing provided by RC Řež).

To elucidate information about the experiments, scoping S/U analyses were performed using the LR-0 models with a simplified version of the new inserted zone. A planar view of the KENO-VI model with a representation of the inserted zone is shown in Figure 11.

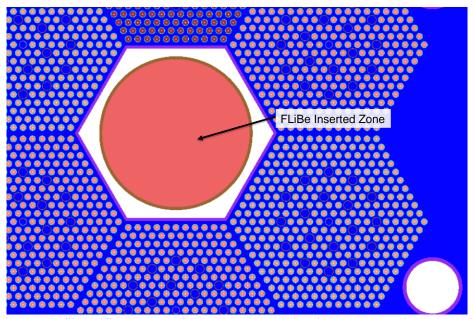


Figure 11. Simplified model of the proposed FLiBe inserted zone in the LR-0.

The FLiBe insertion zone was not a significant potential contributor to eigenvalue bias due to cross sections for the LR-0 experiments. One source of potential uncertainty is due to ⁷Li (n, gamma) representing approximately 0.008% delta-k/k. However, this is a small fraction of the total uncertainty in eigenvalue due to cross sections. The energy dependent sensitivity to ⁷Li (n, gamma) for the LR-0 experiments is shown in Figure 12.

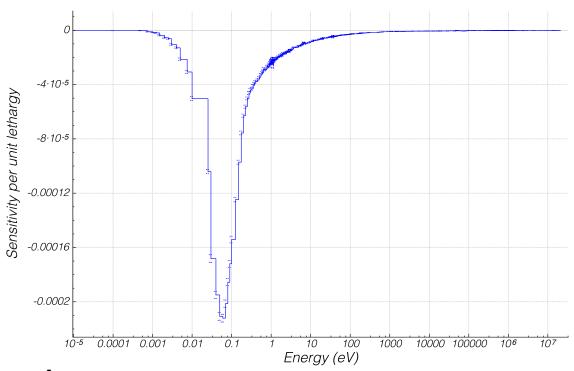


Figure 12. ⁷Li radiative capture sensitivity coefficients for the LR-0 model with the FLiBe insertion.

3. SENSITIVITY AND UNCERTAINTY ANALYSIS OF A TYPICAL FLUORIDE SALT-COOLED HIGH TEMPERATURE REACTOR CONFIGURATION

To maximize usefulness for validation, the experiments in the LR-0 reactor should effectively capture the eigenvalue sensitivity coefficients as a function of energy for FLiBe salts in relevant advanced reactor geometries. The scope of the S/U analysis in this report includes FHRs. FHRs are promising potential options that generate high-temperature heat using a low-pressure, high-power-density system (relative to high temperature gas-cooled reactors), but the technology is relatively immature. FHRs are reactor concepts with a very strong potential for inherent safety, but an FHR has never been built; therefore, directly relevant neutronic benchmarks do not exist.

A 3D assembly model from the AHTR design studies [12] was used to determine eigenvalue sensitivity coefficients. The model is a very detailed 3D assembly with radially reflected boundary conditions but with axial leakage. The assembly model contains both the fuel assembly and the axial reflectors. This is a good approximation of the neutron energy spectrum in a large FHR because the radial neutron leakage in the AHTR is very low. The assembly model contains explicitly defined lattices of tri-isotropic (TRISO) coated fuel particles. A planar slice of the model is shown in Figure 13.

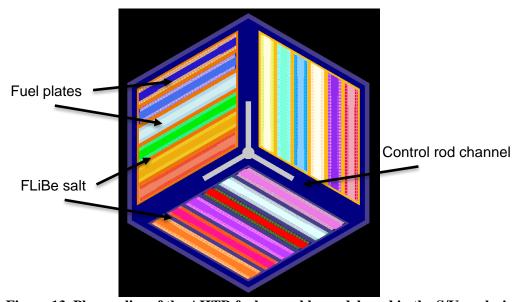


Figure 13. Planar slice of the AHTR fuel assembly model used in the S/U analysis.

The TSUNAMI-3D S/U analysis of the eigenvalue sensitivity coefficients was conducted with FLiBe coolant ⁷Li enrichments (given in weight percent) of 99.95%, 99.995%, and 100.0%. The top contributors to the uncertainty in effective multiplication factor are shown in Table 3 for a ⁷Li enrichment of 99.995%. The most significant potential contributors to eigenvalue bias due to cross sections are similar to other thermal reactors. The main contributors to uncertainty in the FLiBe coolant include ⁷Li radiative capture and elastic scattering. To a lesser extent, ¹⁹F elastic scattering also contributes to the uncertainty.

Table 3. Top contributors to uncertainty in effective multiplication factor from cross section covariance data for the FHR assembly with FLiBe coolant at 99.995% ⁷Li enrichment

Nuclide	Reaction	Covariance w/nuclide	Reaction	Uncertainty in k- _{eff} (%delta-k/k)
Total	N/A	N/A	N/A	$5.22E-01 \pm 4.5E-04$
^{235}U	nubar	^{235}U	nubar	$3.52E-01 \pm 4.39E-05$
^{235}U	n,gamma	^{235}U	n,gamma	$2.33E-01 \pm 9.77E-06$
^{238}U	n,gamma	^{238}U	n,gamma	$2.07E-01 \pm 3.65E-05$
⁷ Li	n,gamma	7 Li	n,gamma	$1.09E-01 \pm 2.94E-06$
^{235}U	fission	^{235}U	n,gamma	$1.03E-01 \pm 1.01E-05$
C	elastic	C	elastic	$9.78E-02 \pm 1.89E-04$
^{238}U	elastic	^{238}U	elastic	$7.65E-02 \pm 1.15E-04$
^{235}U	fission	^{235}U	fission	$6.90\text{E}-02 \pm 9.18\text{E}-06$
^{238}U	elastic	^{238}U	n,gamma	$5.82E-02 \pm 6.60E-05$
⁷ Li	elastic	7 Li	elastic	$4.01E-02 \pm 1.08E-04$
¹⁹ F	elastic	$^{19}\mathrm{F}$	elastic	$2.51E-02 \pm 1.25E-04$
²⁸ Si	n,gamma	²⁸ Si	n,gamma	$2.45E-02 \pm 1.07E-07$
^{235}U	chi	^{235}U	chi	$2.29E-02 \pm 3.03E-04$
⁹ Be	n,2n	⁹ Be	n,2n	$2.25\text{E}-02 \pm 6.18\text{E}-06$
¹⁹ F	n,alpha	$^{19}\mathrm{F}$	n,alpha	$2.03E-02 \pm 1.65E-06$

The contribution of the ⁷Li radiative capture cross section to the overall uncertainty varies as a function of ⁷Li enrichment, as shown in Table 4. The energy dependence of this sensitivity coefficient is shown in Figure 14.

Table 4. Contribution of ⁷Li radiative capture to overall effective multiplication factor uncertainty as a function of ⁷Li-enrichment in FLiBe coolant for the FHR

⁷ Li-enrichment	Uncertainty in k-effective (%delta-k/k)
99.95	$8.80E-02 \pm 1.57E-06$
99.995	$1.09E-01 \pm 2.94E-06$
100.0	$1.24\text{E-}01 \pm 5.11\text{E-}06$

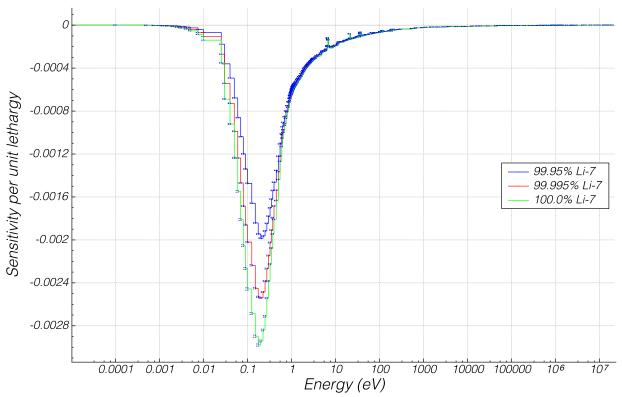


Figure 14. ⁷Li radiative capture sensitivity coefficients for the 3D FHR assembly model.

Another important reaction in FLiBe is ⁶Li (n,t). This reaction is responsible for generating tritium in a FLiBe salt—cooled or –fueled reactor. Therefore, it is vital that the uncertainty in this reaction is understood. The eigenvalue sensitivity coefficients for ⁶Li (n,t) are shown in Table 5 as a function of ⁷Li enrichment. As expected, the results show that the ⁶Li (n,t) contribution to eigenvalue bias due to cross sections is greatest when the ⁷Li-enrichment is least. The results also show significant sensitivity in a ratio with ²³⁵U fission. This is significant because it informs on the void coefficient, which can be positive at lower ⁷Li enrichment and negative at higher ⁷Li enrichment. The energy dependence of this sensitivity is shown in Figure 15.

Table 5. Contribution of ⁶Li (n,t) to overall effective multiplication factor uncertainty as a function of ⁷Li-enrichment in FLiBe coolant

⁷ Li enrichment Nuclide Reaction Covariance Reaction Uncertainty in k-effective					
Li enrichment	Nuchae	Reaction	w/nuclide	Reaction	Uncertainty in k-effective (%delta-k/k)
99.95%	⁶ Li	n,t	⁶ Li	n,t	9.46E-03 ± 1.83E-08
99.95%	⁶ Li	n,t	^{235}U	fission	$-4.35E-03 \pm 1.30E-08$
99.995%	⁶ Li	n,t	^{235}U	fission	$-1.39E-03 \pm 1.51E-09$
99.995%	⁶ Li	n,t	$^6\mathrm{Li}$	n,t	$1.17E-03 \pm 3.44E-10$
100.0%	⁶ Li	n,t	^{235}U	fission	N/A
100.0%	⁶ Li	n,t	⁶ Li	n,t	N/A

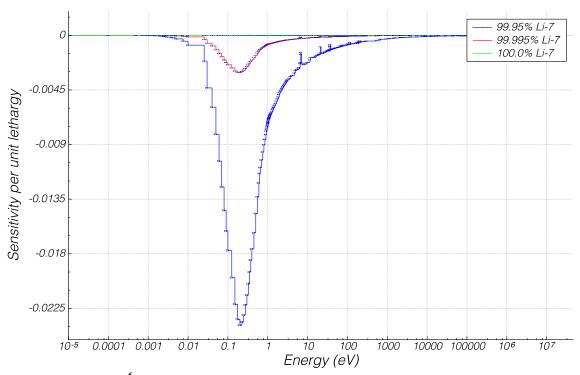


Figure 15. 6 Li (n,t) sensitivity coefficients for the 3D FHR assembly model.

4. SENSITIVITY AND UNCERTAINTY ANALYSIS OF REPRESENTATIVE LIQUID-FUELED MOLTEN SALT REACTOR CONFIGURATIONS

The FLiBe salt experiments in the LR-0 reactor should also effectively capture the eigenvalue sensitivity coefficients as a function of energy for liquid-fueled thermal-spectrum MSRs using FLiBe as the carrier salt for the fuel. Liquid-fueled MSRs offer several unique characteristics that most solid-fueled systems cannot achieve, including online refueling and removal of fission products that could improve resource utilization or decrease potential safety concerns. MSRs also come with several potential technical challenges, including corrosion concerns and tritium containment. Despite having the MSRE as an early engineering-scale demonstration reactor [13], MSRs remain relatively immature as a reactor technology. Significant public and private interest has surfaced recently in liquid-fueled MSR concepts due to their potential benefits and wide range of possible design space and operational modes. These recent efforts, many of which are privately funded design and technology development efforts at startup companies, cover a range of MSR designs, including options in the fuel (uranium, thorium, or recycled spent nuclear fuel from existing light water reactors), neutron energy spectrum (thermal, intermediate, fast, or mixed spectrum), and fuel cycles approaches (open fuel cycle with once-through or limited recycle, or a closed fuel cycle with continuous recycle). In particular, thorium-fueled MSRs are of potential interest in the thermal neutron energy spectrum [15], as well as the intermediate or fast neutron energy spectrum [16], depending upon specific design choices and missions.

MSR application models used for this S/U analysis effort were built using an existing 2D unit cell model of a single-zone one-fluid MSR based on the MSBR. This model was adapted to use 3D geometry and CE cross sections and then modified to analyze two representative MSR systems of interest: (1) a thermal-spectrum MSR fueled with low-enriched uranium (LEU) operating in a once-through fuel cycle, and (2) a thermal-spectrum MSR using thorium fuel with continuous recycle of ²³³U produced in the system (Th/²³³U). The simple 2D unit cell model of a salt flow channel in a graphite block misses possible benefits of going to a two-zone system with different neutron energy spectra in the zones to enhance breeding or burning. However, this approach provides quick scoping calculations and should be a reasonable approximation of the neutron energy spectrum in a large MSR using a similar fuel and actinide management strategy. The overall geometry for an example unit cell from these application models, shown below in Figure 16, remains the same as the base model, though values and material compositions may vary for specific parameters and regions.

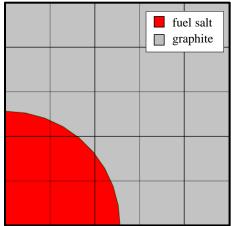


Figure 16. Unit cell geometry for an MSR application model, reproduced from Reference 15.

4.1 LEU-FUELED MSR

The LEU-fueled MSR application model offers the highest degree of similarity to the LR-0 FLiBe experiments of the liquid-salt systems considered in this work and is therefore examined first. The eigenvalue sensitivity coefficients of the LEU MSR model were calculated using TSUNAMI-3D S/U at four different ⁷Li enrichments (in weight percent) in the FLiBe carrier salt: 99.95%, 99.995%, 99.995%, and 100.0%. Table 6 lists the total uncertainty in effective multiplication factor for the 99.995% -enriched ⁷Li case along with the top 15 contributors, Similar to the LR-0 and FHR S/U analyses, the LEU MSR results indicate that ²³⁵U and ²³⁸U are the most significant potential contributors to eigenvalue bias due to cross sections. As with the FHR application model, the main salt-specific contributor to uncertainty is ⁷Li radiative capture with ⁷Li elastic scattering and ¹⁹F elastic scattering making smaller contributions. These LEU MSR results find ¹⁹F elastic scattering of higher importance than ⁷Li elastic scattering, which is opposite of the order seen in FHR analyses above, though both cases have relatively similar values. The LEU MSR results also indicate that elastic scattering in graphite is a slightly larger contributor than was seen in the FHR analysis above, followed closely by radiative capture in graphite, which did not show up as a top contributor for the FHR model. Overall, these results show that FHR and LEU MSR models both indicate that ⁷Li is the top salt-specific contributor. However, minor differences do occur in the smaller contributions from other reactions in ⁷Li, ¹⁹F, and graphite due to reasons including differences in neutron energy spectrum and nuclide concentration.

Table 6. Top contributors to uncertainty in effective multiplication factor from cross section covariance data for the LEU MSR model using FLiBe salt with 99.995% ⁷Li enrichment

Nuclide	Reaction	Covariance with nuclide	Reaction	Uncertainty in k-effective (% Ak/k)
Total	N/A	N/A	N/A	0.55412 ± 0.00082
^{235}U	nubar	^{235}U	nubar	$3.74E-01 \pm 1.32E-04$
^{238}U	n,gamma	^{238}U	n,gamma	$2.61E-01 \pm 5.14E-05$
^{235}U	n,gamma	^{235}U	n,gamma	$1.96E-01 \pm 2.02E-05$
^{235}U	fission	^{235}U	n,gamma	$1.21E-01 \pm 2.96E-05$
⁷ Li	n,gamma	⁷ Li	n,gamma	$1.10\text{E-}01 \pm 6.04\text{E-}06$
C	elastic	C	elastic	$1.06E-01 \pm 6.45E-04$
C	n,gamma	C	n,gamma	$9.29E-02 \pm 2.96E-06$
^{235}U	fission	^{235}U	fission	$9.20E-02 \pm 3.34E-05$
^{238}U	elastic	^{238}U	n,gamma	$3.92E-02 \pm 6.59E-05$
^{238}U	elastic	^{238}U	elastic	$3.70E-02 \pm 1.18E-04$
19 F	elastic	¹⁹ F	elastic	$2.14\text{E}-02 \pm 2.06\text{E}-04$
^{238}U	n,n'	^{238}U	elastic	$1.86E-02 \pm 1.21E-04$
⁷ Li	elastic	⁷ Li	elastic	$1.69E-02 \pm 1.25E-04$
^{235}U	chi	^{235}U	chi	$1.34\text{E-}02 \pm 3.18\text{E-}04$
²³⁸ U	nubar	²³⁸ U	nubar	$1.20E-02 \pm 2.37E-06$

Table 7 shows how the contribution of ⁷Li radiative capture to the overall uncertainty in effective multiplication factor varies as a function of ⁷Li enrichment for the LEU MSR model. Figure 17 shows the energy dependence of the ⁷Li radiative capture sensitivity coefficient as a function of ⁷Li enrichment for the LEU MSR model.

Table 7. Contribution of ⁷Li radiative capture to overall effective multiplication factor uncertainty as a function of ⁷Li enrichment in LEU MSR model

⁷ Li-enrichment (wt %)	Uncertainty in k-effective (%∆k/k)
99.95	$1.0195\text{E-}01 \pm 5.8\text{E-}06$
99.995	$1.1029\text{E-}01 \pm 6.0\text{E-}06$
99.9995	$1.1142E-01 \pm 6.1E-06$
100.0	$1.1140E-01 \pm 6.3E-06$

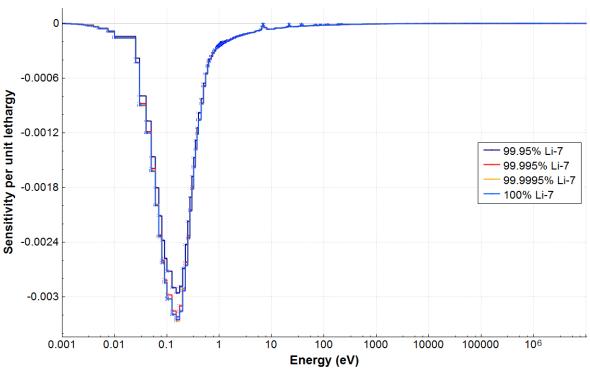


Figure 17. ⁷Li radiative capture sensitivity coefficients for the 3D LEU MSR model.

Another potentially important reaction in the LEU MSR model is ⁶Li (n,t). The eigenvalue sensitivity coefficients for ⁶Li (n,t) are shown in Table 8 as a function of ⁷Li enrichment for the LEU MSR model. As expected, the contribution of ⁶Li (n,t) to eigenvalue bias is greatest when the ⁷Li enrichment is least, and thus ⁶Li content is greatest. The results also show sensitivity to the covariance between ⁶Li (n,t) and ²³⁵U fission, which could relate to reactivity coefficients and thus operational and safety factors. Figure 18 shows the energy dependence of the self-covariant sensitivities as the different ⁷Li enrichments.

Table 8. Contribution of ⁶Li (n,t) to overall effective multiplication factor uncertainty as a function of ⁷Li-enrichment in LEU MSR model

⁷ Li enrichment	⁶ Li content	Nuclide	Reaction	Covariance	Reaction	Uncertainty in k-effective
(wt %)	(wt %)			w/nuclide		(% ∆k/k)
99.95	0.05	⁶ Li	n,t	⁶ Li	n,t	$1.10E-02 \pm 6.8E-08$
99.95	0.05	⁶ Li	n,t	^{235}U	fission	$-3.87E-03 \pm 2.6E-08$
99.995	0.005	⁶ Li	n,t	⁶ Li	n,t	$1.19E-03 \pm 7.1E-10$
99.995	0.005	⁶ Li	n,t	^{235}U	fission	$-1.17E-03 \pm 2.7E-09$
99.9995	0.0005	⁶ Li	n,t	⁶ Li	n,t	$1.20E-04 \pm 7.1E-12$
99.9995	0.0005	⁶ Li	n,t	^{235}U	fission	$-3.65E-04 \pm 2.8E-10$
100	0	⁶ Li	n,t	⁶ Li	n,t	N/A
100	0	⁶ Li	n,t	^{235}U	fission	N/A

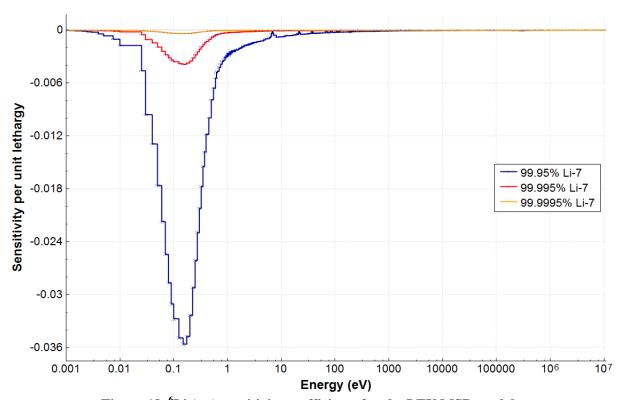


Figure 18. ⁶Li (n,t) sensitivity coefficients for the LEU MSR model.

The total sensitivity values were verified for the LEU MSR model with 99.95%-enriched ⁷Li using direct perturbation of nuclide densities for ⁶Li, ²³⁵U, and the graphite moderator in independent perturbation calculations for each nuclide. Similar total sensitivities were found for the direct perturbation and the TSUNAMI-3D calculation.

4.2 Th/²³³U-FUELED MSR

The Th/ 233 U MSR model differs substantially from all previous LR-0, FHR, and LEU MSR models in its use of thorium as a fertile material and 233 U as a primary fissile material. Consequently, TSUNAMI-3D S/U analysis of the eigenvalue sensitivity coefficients found some significant differences in results due to

the change in fertile and fissile actinide species. The salt modeled for these calculations represents an unirradiated salt (no fission products or activation products) with heavy metal ratios intended to support slight net breeding of fissile material, and thus had a low 233 U content (about 0.3 mol% UF₄ in the salt) with a higher thorium content (about 12 mol% ThF₄ in the salt).

TSUNAMI-3D calculations were performed using CE cross sections for the Th/²³³U MSR model to identify the top contributors to the uncertainty in effective multiplication factor, which are shown in Table 9 for the 99.995%-enriched ⁷Li case. The biggest contributors to eigenvalue uncertainty in the fuel salt include ²³³U nubar and fission, ²³²Th radiative capture and elastic scattering, ⁷Li radiative capture, and natural carbon (C) radiative capture and elastic scattering. Smaller contributions also come from ¹⁹F radiative capture and even the ²³³U chi distribution. These contributors highlight the fact that liquid-fueled systems using Th/²³³U fuel will have some significant contributors that will not be present in LR-0 (e.g., ²³³U and ²³²Th) but will also have significant contributors (e.g., ⁷Li and ¹⁹F) for which LR-0 experiments may help provide experimental data. Increased contributions from the graphite moderator, ¹⁹F, and covariance between reactions such as ²³³U fission and ²³³U radiative capture appear to indicate that there may be higher uncertainty contributions from the salt and that there may be significant differences in contributions from the fuel species due to underlying uncertainties in their nuclear data. Figure 19 shows the energy dependence of some of the top contributors in the same Th/²³³U MSR model, with peak sensitivities occurring around a neutron energy level of 0.2 eV.

Table 9. Top contributors to uncertainty in effective multiplication factor from cross section covariance data for the Th/²³³U MSR model with 99.995% ⁷Li enrichment in FLiBe carrier salt

Nuclide	Reaction	Covariance with nuclide	Reaction	Uncertainty in k-effective (% Δk/k)
Total	N/A	N/A	N/A	0.74734 ± 0.00027
^{233}U	nubar	^{233}U	nubar	$4.83E-01 \pm 7.13E-05$
²³² Th	n,gamma	²³² Th	n,gamma	$4.50E-01 \pm 5.14E-05$
^{233}U	fission	^{233}U	fission	$2.04E-01 \pm 6.35E-05$
⁷ Li	n,gamma	⁷ Li	n,gamma	$2.00E-01 \pm 5.42E-06$
C	n,gamma	C	n,gamma	$1.56E-01 \pm 2.49E-06$
^{233}U	n,gamma	^{233}U	n,gamma	$1.07E-01 \pm 1.76E-06$
²³² Th	elastic	²³² Th	elastic	$3.75E-02 \pm 7.74E-05$
C	elastic	C	elastic	$3.54E-02 \pm 2.08E-04$
19 F	n,gamma	¹⁹ F	n,gamma	$2.94E-02 \pm 1.17E-07$
^{233}U	fission	^{233}U	n,gamma	$2.14E-02 \pm 1.58E-06$
²³² Th	elastic	²³² Th	n,gamma	$1.85E-02 \pm 6.25E-05$
¹⁹ F	elastic	¹⁹ F	elastic	$1.82E-02 \pm 6.47E-05$
¹⁹ F	n,alpha	¹⁹ F	n,alpha	$1.51E-02 \pm 6.31E-07$
C	n,n'	C	n,n'	$1.36E-02 \pm 3.43E-05$
²³³ U	chi	²³³ U	chi	$1.22E-02 \pm 4.71E-05$

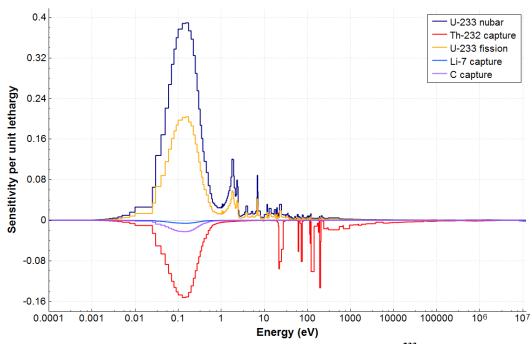


Figure 19. Sensitivity coefficients for top contributors in Th/²³³U MSR model.

Overall trends shown for variations in results at different ⁷Li enrichments in the FHR and LEU MSR models hold true in the Th/²³³U MSR model as well, though as expected specific numerical results and ratios vary. Therefore, results are not shown or discussed for these different ⁷Li enrichments in the Th/²³³U MSR model because no additional insight would be gained.

5. SIMILIARITY ASSESSMENT OF LR-0 EXPERIMENTS TO APPLICATION MODELS

One key objective of this S/U analysis work was to assess how well the LR-0 FLiBe experiments capture the sources of potential bias due to nuclear data uncertainty in FHR and MSR application models of interest. Both quantitative and qualitative approaches exist to complete this assessment.

An initial effort to address this issue, shown in Figure 20, compared the normalized sensitivity profiles in the LR-0 experiment and the FHR application model for the ⁷Li (n,gamma) reaction. This comparison illustrates a significant spectral shift between the water-moderated LR-0 and the graphite-moderated FHR application model, which impacts the energy dependence of the sensitivity profiles. However, the general shape and distribution of the sensitivity appears similar between the two models.

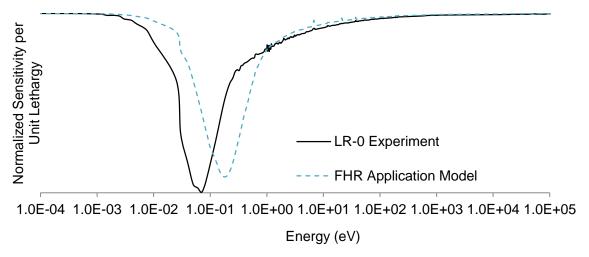


Figure 20. Normalized ⁷Li radiative capture sensitivity coefficients showing spectral shift of sensitivity between water moderated LR-0 and graphite moderator FHR application model.

Figure 21 provides a direct comparison of the energy-dependent sensitivity to ⁷Li radiative capture calculated for the September 2016 LR-0 FLiBe experiments to the sensitivities calculated in the FHR, LEU MSR, and Th/²³³U MSR application models. All calculations used TSUNAMI-3D with CE cross sections. The FHR and MSR models shown used a lithium enrichment of 99.995% ⁷Li in FLiBe. This comparison shows that the application models are more sensitive to ⁷Li radiative capture than the LR-0 FLiBe experiment models. In addition, the energy at which each sensitivity profile peaks varies; the LR-0 FLiBe experiment sensitivity peaks at lower neutron energy levels than the application models.

Differences between results for the application models exist, too. The FHR and LEU MSR models exhibit similar peak sensitivity magnitudes, with the LEU MSR peak being about 25–30% greater, but the Th/²³³U MSR hits a peak sensitivity magnitude about twice as great. Significant spectral variation between the three application models also occurs, likely primarily due to differences in fuel-to-moderator ratios and specific material cross sections. The sensitivity profile for the Th/²³³U MSR peaks at neutron energies considerably more thermal than the FHR model, with the LEU MSR results falling in between.

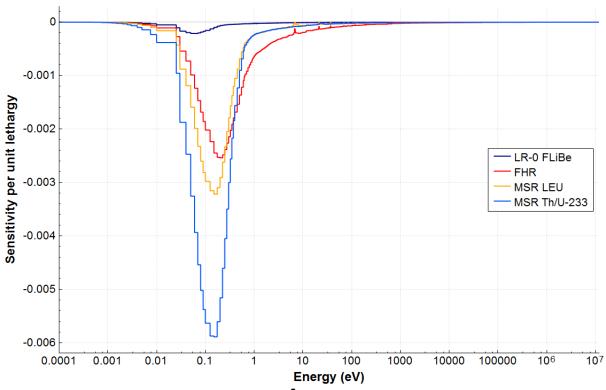


Figure 21. Comparison of energy-dependent ⁷Li radiative capture sensitivity coefficients from models for LR-0 FLiBe experiment, FHR, LEU MSR, and Th/²³³U MSR.

Additional efforts assessing the similarity between LR-0 experiments and application models used TSUNAMI-IP to compare sensitivity results obtained from TSUNAMI-3D calculations for the LR-0, FHR, and LEU MSR models. TSUNAMI-IP reads in sensitivity data files from TSUNAMI-3D calculations and calculates a similarity index (c_k) that aids in quantitatively assessing the similarity of an experiment to an application model. A similarity index of 1.0000 would indicate perfect similarity.

Numerous TSUNAMI-IP calculations were performed to assess the similarity between LR-0 experiments and application models. Models of LR-0 experiments included a "clean" LR-0 configuration with no salt and the LR-0 FLiBe experiments described in Section 2.3. All FHR and MSR models selected used lithium enriched to 99.995% ^7Li in FLiBe. Table 10 provides the similarity index calculated by TSUNAMI-IP for numerous combinations considering different models as the experiment or application model. The LR-0 models appear to be extremely similar to each other (c_k=0.9961). The LR-0 FLiBe experiment appears to be somewhat similar to the FHR and LEU MSR models, with c_k values of 0.6402 and 0.6942, respectively. The FHR and LEU MSR models also appear to be quite similar. However, the LR-0 FLiBe experiment appears to lack almost any similarity to the Th/ 233 U MSR application model (c_k=0.0054), and the LEU MSR application model is only slightly more similar to the Th/ 233 U MSR application model (c_k=0.1394). This highlights the importance of fuel materials in driving overall similarity of an experiment to an application.

Table 10. Similarity indices calculated using TSUNAMI-IP using different combinations of LR-0,

FHR, and MSR models as the experiment and application. Application Experiment **Similarity Index** $(\mathbf{c}_{\mathbf{k}})$ LR-0 "clean" 0.9961 ± 0.0035 LR-0 FLiBe LR-0 FLiBe FHR 0.6402 ± 0.0013 LR-0 FLiBe MSR LEU 0.6942 ± 0.0036 MSR Th/233U LR-0 FLiBe 0.0054 ± 0.0001 **FHR** MSR LEU 0.8790 ± 0.0028 MSR Th/233U MSR LEU 0.1394 ± 0.0011

The results in this section from Figure 20, Figure 21, and the TSUNAMI-IP similarity index (c_k) values discussed above all indicate that existing LR-0 FLiBe experiments provide some benefit for salt reactor neutronics calculations. However, they may not provide similar enough sensitivities to specific nuclides and reactions to be of direct relevance to FHR and MSR application models using LEU fuel. The sensitivity differences observed included both spectral effects due to the LR-0 reactor being watermoderated and sensitivity magnitude effects driven by the quantity of FLiBe inserted and its location.

In addition, it should be noted that existing LR-0 FLiBe experiments are likely of little direct relevance to FHR or MSR application models using fuels with thorium and/or ²³³U; the extremely low similarity index between the LR-0 FLiBe experiment and the Th/²³³U MSR application model strongly indicates that water-moderated LEU experiments will not be of high value when trying to identify nuclear data biases in graphite-moderated, salt-cooled applications models using Th/²³³U fuel. This result was expected, but it remains an important consideration for applications work and could motivate new critical experiments in the future.

Future critical experiments using salt at LR-0 benefit from the use of the S/U analysis methods described in this report to help inform their experimental designs and improve their similarity to application models.

6. SUMMARY

This final report details the collaboration on the MSRE FLiBe experiments between RC Řež and ORNL during 2016. In May 2016 and September 2016, delegations from the United States visited the Czech Republic. The May visit included observations of experimental operations at the LR-0 reactor and collaborative discussions on enhancements that S/U analysis can provide to LR-0 experiments. The September visit focused on the FLiBe experiments and discussing the preliminary findings of this study.

A 3D model of the LR-0 reactor was developed using the SCALE code system. Scoping S/U analyses were performed for several example configurations of the LR-0. These S/U analyses show similar sources of potential bias in LR-0 relative to other light water reactors, with approximately 0.6% delta-k/k uncertainty in the neutron multiplication factor.

Application models were adapted for S/U analysis of FHR and MSR concepts using geometries representative of the AHTR and MSBR designs. These models were used to perform initial scoping S/U analyses for FHR and MSR concepts. One objective of the LR-0 experiments should be to generate experimental configurations that reproduce these sensitivities. The most significant potential source of bias within the FLiBe salt in FLiBe-cooled and -fueled configurations is radiative capture in ⁷Li. This indicates that previous RC Řež experiments using FLiNa salt should be considered candidate benchmarks for these application models and should be evaluated for suitability using S/U analysis.

There were differences in the energy dependence of the key FLiBe sensitivity coefficients in the LR-0 and in the advanced reactor application models. These were due primarily to the different neutron energy spectral characteristics related to neutron moderation in water versus graphite.

The key finding of this work is that, for both solid- and liquid-fueled fluoride salt reactors, radiative capture in ⁷Li is the most significant contributor within the FLiBe salt to potential bias from nuclear data in neutronics calculations.

7. REFERENCE

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APPENDIX A. SUMMARY OF THE MAY 2016 COLLABORATIVE MEETING BETWEEN ORNL AND RC ŘEŽ

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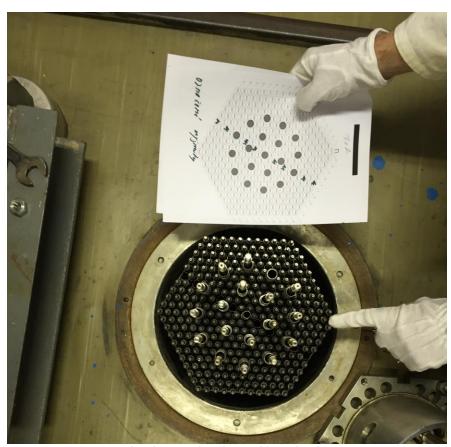
This appendix provides a brief overview of ORNL staff visit to RC Řež in May 2016. Donald E. Mueller, Nicholas R. Brown, and Jeffrey J. Powers of ORNL in Oak Ridge, Tennessee, visited the RC Řež in the Czech Republic. The visit was conducted from Tuesday, May 17, 2016, to Thursday, May 19, 2016. The visit included tours of several key facilities of RC Řež. The visit enabled ORNL participants to observe critical experiments, develop a better understanding of the capabilities and limitations of the facility, and work with the RC Řež researchers to potentially enable development of enhanced experiment designs.

The meetings on Tuesday, May 17, 2016, included observations of several critical experiments with graphite, including the measurement of the axial profile of fission density of the driver core using gamma-scanning equipment. Donald Mueller and Nicholas Brown met with Jan Uhlíř (Fluorine Chemistry Department), Michal Košťál (scientist at LR-0), Vlastimil Juricek (head of Řež Reactors Operation), and Ján Milčák (head of LR-0 Operations). Discussions included general opportunities for collaboration and other synergies, as well as technical discussion with Michal Košťál about gamma scanning and experimental uncertainties in LR-0. Donald Mueller engaged in a discussion with Michal Košťál about the potential applications of S/U analysis tools, which led to discussion about planning for future collaborations and opportunities for enhanced experiment design.

On Wednesday, May 18, 2016, Donald Mueller presented a seminar on S/U analysis and its impact on critical experiment design, and Nicholas Brown presented a seminar on the development of a point design for a fluoride high temperature salt-cooled reactor and other US advanced reactor activities. The seminar had approximately 12 attendees, including Miroslav Hrehor, director of the Safety Research Section. The seminar resulted in productive discussions on several topics. The ORNL participants observed additional operations at LR-0 and engaged in a consensus-building discussion about the design of a canister for future experiments using the MSRE FLiBe salt obtained by Czech Republic from the United States. There were also detailed discussions with facility staff about LR-0 modeling approaches.

In the afternoon, ORNL participants toured the RC Řež Fluorine Chemistry Laboratory and engaged in productive discussions on fluoride volatility (relevant to advanced reactor and sustainable fuel cycles), FLiBe salt, and electrochemistry.

Meetings on Thursday, May 19, 2016, included detailed discussion of modeling issues of the LR-0 reactor, including one of the main LR-0 modelers, Evžen Losa. Resolution of these issues enabled unification of preliminary ORNL models of the LR-0 reactor with the physical system, as well as the RC Řež reactor physics models. One example included identification of the physical orientation of the guide tube locations in the assemblies relevant for the past experiments related to molten salt and graphite and the planned experiments with MSRE FLiBe, as shown in the photograph below. These in-person discussions answered questions and enabled modeling improvements for both sides of the collaboration.



Identification of LR-0 assembly guide tube orientation.

The participants formulated a strategic near-term plan to collaborate on the modeling and S/U analysis of the LR-0 reactor, particularly the experiments with MSRE FLiBe salt planned for the September 2016 time frame. These plans included specific interactions throughout 2016 focused on the design, analysis, and conduct of the FLiBe experiments.

APPENDIX B. SUMMARY OF THE SEPTEMBER 2016 COLLABORATIVE MEETING BETWEEN ORNL AND RC ŘEŽ

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On September 27, 2016, Nicholas Brown and Jeffrey Powers of Oak Ridge National Laboratory (ORNL) in Oak Ridge, Tennessee, visited the Centrum výzkumu Řež (Research Centre Řež, or RC Řež) in the Czech Republic as part of an ongoing collaboration between the United States and Czech Republic focused on molten salt reactor technology. This collaboration was initiated by a Memorandum of Understanding (MOU) between the Czech Republic and United States that was signed in December 2012. In 2013, about 75kg of FLiBe coolant salt originally from the Molten Salt Reactor Experiment (MSRE) was transferred from ORNL to RC Řež as part of the ongoing collaboration.

This visit was the second meeting at RC Řež as part of a collaboration currently focused on applying ORNL sensitivity and uncertainty (S/U) analyses to RC Řež experimental work. The RC Řež researchers recently performed several experiments with a FLiBe coolant salt target in the LR-0 reactor to determine if current nuclear data for FLiBe salt performs well enough to enable simulations to match the measured critical configurations. In parallel, the ORNL researchers performed S/U analyses using the SCALE package to analyze those LR-0 experiments and assess how current or future salt experiments at LR-0 could be used to develop confidence in conceptual design application models of interest for design and operation of both solid-fueled fluoride salt-cooled high-temperature reactor (FHR) and liquid-fueled molten salt reactor (MSR) concepts.

The three main objectives for this meeting were (1) to discuss recent progress made by both organizations, (2) to agree upon remaining work to be performed during 2016 under existing funding at both RC Řež and ORNL, and (3) to identify and discuss possible areas for future collaboration between ORNL and RC Řež in 2017 if each organization's sponsoring agencies provide additional funding.

The morning began with the researchers participating in a high-level meeting to celebrate the ongoing collaboration in civilian nuclear energy research and development between the United States and Czech Republic over the past few years. The meeting included a presentation by Jan Uhlíř (RC Řež) giving an overview of this current collaborative project in MSR technologies. There were about 20 participants at the meeting including senior laboratory management at Řež, representatives from Czech government ministries, representatives from the US Embassy in Prague, including The Honorable Andrew H. Schapiro (US Ambassador to the Czech Republic), and researchers from RC Řež and ORNL. The photo below shows some of the participants.



First row: Jeffrey Powers (ORNL), Martin Ruščák (Director of CV Řež), Andrew Schapiro (US Embassy Prague), Miroslav Horák (Acting Director of ÚJV Řež), Nicholas Brown (ORNL), Michal Košťál (RC Řež). Second row: Jan Uhlíř (RC Řež), Arnošt Marks (Deputy of Czech Vice Premier for Science), Hana Obrusníková (US Embassy Prague), Daneš Burket (Energy R&D Director of CV Řež), Vlastimil Juříček (Reactor Operation Director of CV Řež), Evžen Losa (RC Řež).

After the conclusion of the short ceremony, a technical meeting between ORNL (Brown, Powers) and RC Řež (Košťál, Losa) was conducted for the rest of the morning. Each organization presented some of their recent progress. For RC Řež, this included showing results from recent LR-0 experiments using a central container of MSRE FLiBe salt and discussing what conclusions might be drawn from those experiments regarding the adequacy of existing nuclear data and computational models. Košťál and Losa also showed a variety of recent publications produced using data from LR-0 experiments to illustrate the broad range of facility capabilities and highlight relevant areas of research that might overlap with current or future work in this collaboration. Discussions led by ORNL focused on S/U analysis to identify potential sources of bias in fluoride salt reactor models due to nuclear data and assess how those potential biases might be reduced using well-designed experiments at the LR-0 reactor. The meeting included specific discussion of ORNL efforts to model the LR-0 reactor using SCALE S/U analysis tools (mainly TSUNAMI-3D) and gauging the potential relevance of energy-dependent sensitivities in the LR-0 experiments to the calculated uncertainties and sensitivities from representative FHR and MSR application models.

The morning meeting progressed to a discussion of the remaining work to be performed during 2016 using existing funding at each organization. Based on the amount of funds remaining and the significant progress already achieved, both organizations agreed that work would mostly focus on concluding existing efforts and publishing the research. RC Řež will finish the current LR-0 FLiBe experiments by gathering additional data, reviewing ORNL's model of LR-0, and summarizing the results from all of the FLiBe experiments. Afternoon discussions also clarified that experimentalists at RC Řež will characterize the MSRE FLiBe salt using various mass spectrometry techniques (including Secondary Ion Mass Spectrometry) to precisely determine the lithium enrichment level in the salt (mass fractions of ⁶Li and ⁷Li in lithium) and identify any other significant trace contaminants in the salt. ORNL will complete the S/U analyses of applications models and LR-0 configurations by refining the models, making a final rerun of all necessary calculations using the best versions of the models and nuclear data available, and documenting its work. Two joint publications will be pursued. One journal article, to be led by RC Řež, will focus on the FLiBe and Teflon® experiments in LR-0 (including spectral analysis); ORNL will

contribute S/U analysis of LR-0 and preliminary application modeling for one FHR case. A second journal article, to be led by ORNL, will focus on S/U analysis of the applications models and tying the uncertainties of the FHR/MSR models back to sensitivities in the LR-0 experiments; RC Řež will contribute some application model S/U analysis of its own for other concepts.

Several possible areas of future work were identified and discussed into the afternoon, including (1) enhancing the sensitivity to FLiBe salt in LR-0 experiments using alternate core configurations or slight changes to the existing configuration (e.g., adding another salt vessel in the reflector), (2) submitting a benchmark proposal to the OECD/NEA based on FLiBe salt experiments in LR-0, and (3) investigating the adequacy of current nuclear data for graphite as a moderating material. RC Řež researchers also informed ORNL that plans call for the current LR-0 configuration being used for FLiBe experiments to be disassembled sometime around October 12 through October 14, after which it will likely be about a year before the same FLiBe experiment configuration would be set up again in LR-0 due to other work being performed. Jan Uhlíř joined the group for portions of the afternoon discussion, as seen in the photo below.



From left to right: Evžen Losa, Michal Košťál, Jan Uhlíř, Nicholas Brown, Jeffrey Powers.

Substantial information exchange and progress was achieved during this meeting, with ORNL and RC Řež participants all expressing that they were pleased with the current status and near-term direction of the collaboration. Current project plans and funding indicate that this specific collaboration between the US and Czech Republic on MSR technologies will end in December 2016. However, several possible areas of worthwhile future collaboration were identified that could be performed if sponsoring agencies provide additional funding to each organization.