NEUTRONICS PHENOMENA IMPORTANT IN MODELING AND SIMULATION OF LIQUID-FUEL MOLTEN SALT REACTORS

David J. Diamond
Brookhaven National Laboratory
Upton, NY 11973-5000
diamond@bnl.gov

Nicholas R. Brown
Pennsylvania State University
University Park, PA 16802
nrb26@psu.edu

Richard Denning
Consultant
Columbus, Ohio 43220
denningrs.8@gmail.com

Stephen Bajorek
U.S. Nuclear Regulatory Commission
Washington, DC 20555
stephen.bajorek@nrc.gov

ABSTRACT

This paper discusses liquid-fuel molten salt reactors, how they will operate under normal, transient, and accident conditions, and the results of an expert elicitation to determine the corresponding neutronic phenomena important to understanding their behavior. Identifying these phenomena will enable the U.S. Nuclear Regulatory Commission (NRC) to develop or identify modeling functionalities and tools required to carry out confirmatory analyses that examine the validity and accuracy of applicant's calculations and help determine the margin of safety in plant design. NRC frequently does an expert elicitation using a Phenomena Identification and Ranking Table (PIRT) to identify important modeling phenomena. However, few details about the design of these reactors and the sequence of events during accidents are known, so the process used was considered a preliminary PIRT. A panel met to define phenomena that would need to be modeled and considered the impact/importance of each phenomenon with respect to specific figures-of-merit (FoMs) (e.g., power distribution, fluence, kinetics parameters and reactivity). Each FoM reflected a potential impact on radionuclide release or loss of a barrier to release. The panel considered what the path forward might be with respect to being able to model the phenomenon in a simulation code. Results are explained for both thermal and fast spectrum designs.

KEYWORDS
Liquid-fuel, molten-salt, neutronics modeling.

1. INTRODUCTION

1.1 Background

The U.S. Nuclear Regulatory Commission (NRC) is preparing for the future licensing of advanced reactors. These reactors will be very different from the light water reactors (LWRs) that are currently used to provide electricity generation in the U.S. In particular, many of them will use gas, liquid metal, or molten salt as a coolant rather than water. NRO has developed a vision and strategy document [1] that outlines the tasks that must be undertaken to advance technical and regulatory readiness and related communications for these non-LWRs. That document is supported by an implementation plan [2] that covers the actions to be taken in the next five years based on six basic strategies.

Strategy 2 of the plan is to "acquire/develop sufficient computer codes and tools to perform non-LWR regulatory reviews." As part of the NRC evaluation of a new design, confirmatory safety analyses are performed to understand the validity and accuracy of computational methods being used by licensees, the sensitivity of results to uncertainties, and the safety margin under varying conditions from normal operation to design-basis and beyond design-basis accidents. The immediate priority is to identify a set of existing computational tools and functional needs that must be developed to model neutronics, heat transfer, and fluid dynamics. This will allow for time-dependent simulations in the fuel and coolant of neutron flux, power density, temperature, flow rate, and pressure for these advanced non-LWRs.

The intent is to consider all designs under consideration in the U.S. that might result in a license or design submittal to the NRC in the next decade. Of the three types of non-LWR designs mentioned above, the most pressing needs with respect to Strategy 2 are with molten salt cooled reactors (MSRs) where developing simulation tools might be most challenging. This includes reactors with solid fuel or fuel dissolved in the salt. Since companion studies of solid-fuel MSRs exist [3, 4], the present study is limited to liquid-fuel MSRs. This paper, based on a more detailed report [5], discusses neutronics phenomena; a companion paper [6] discusses thermal-hydraulic phenomena.

1.2 Objectives

The objective of this study was to start the process outlined in Strategy 2 by considering the needs for the modeling of neutronics in liquid-fuel MSRs. Due to the preliminary nature of the information available on these MSR designs, the focus was the primary system and not secondary or tertiary heat transport systems or auxiliary systems for residual heat removal. The accident phenomena of interest are for events leading up to the potential failure of the primary system boundaries, including the potential melting of a freeze plug if present. Accidents associated with fuel processing that might be an integral part of a liquid-fuel MSR plant are not considered.

The recommendation of specific computer tools for use by the NRC is not a part of this work. However, the findings in this report can be used to facilitate a functional needs assessment and examine the applicability of NRC's TRACE and PARCS codes as well as several of the U.S. Department of Energy's codes for application to MSRs.

2. METHODOLOGY

In assessing the adequacy of computer codes to address accident phenomena and to identify areas of needed improvement, the NRC has frequently followed a process known as Code, Scaling, Applicability and Uncertainty (CSAU). CSAU is a structured process that helps define code capability and ensures that physical processes important to an accident scenario are properly taken into account. One of the first steps of CSAU involves development of a Phenomena Identification and Ranking Table (PIRT) [7]. The

PIRT process involves a review of the design for particular events and identification of the physical phenomena expected to be most dominant. In development of the PIRT a group of technical experts identifies the phenomena and ranks the state of knowledge of each phenomenon and its importance to safety-related consequences. The phenomena with high importance and low knowledge level then become a priority for future research, which may be analytical or experimental.

The PIRT cannot only be useful in helping to define new simulation tools, but it can also provide guidance for reviews of an applicant's evaluation model and analysis methods. The physical processes identified in the PIRT as important must also be addressed by an applicant.

Normally, a PIRT is carried out with knowledge of an identified system design and specific transients/accidents already identified, in particular the licensing basis events and risk-significant beyond design-basis events. The state of knowledge of candidate molten salt reactor designs and the selection of licensing basis events is not yet at that stage of development. A preliminary PIRT-like activity, referred to as a "pre-PIRT" in this report, was carried out to assist the NRC in planning the next steps toward having a simulation capability.

The pre-PIRT was completed for a range of potential design concepts, rather than a specific design as discussed in Section 3. The panel[a] first considered normal operating conditions, which establish the initial conditions for accident scenarios. They then considered generic transient conditions, such as reactivity insertion accidents, flow coast-down accidents, and loss of primary system heat removal as discussed in Section 4.

The results, in Sections 5 and 6, are the physical processes that must be modeled to have a viable simulation capability. To identify the phenomena and evaluate the significance of deficiencies in the current ability to model them, a set of figures-of-merit (FoMs) was established by the experts. The concern of the NRC is either the margin to an acceptance criterion or with the magnitude of release of radioactive material and the associated radiological dose to the public. Thus, in developing figures-of-merit, the panel recognized that each FoM should reflect potential impact on radionuclide release or loss of a barrier to release, even though the mechanisms of radionuclide release and transport were not considered in the pre-PIRT. Each of the identified phenomena is evaluated with regard to its impact on these figures-of-merit.

The panel also discussed what the next steps might be for obtaining an adequate level of understanding for each phenomenon to support confirmatory analysis. This includes identifying existing applications where the phenomenon is already modeled, suggestions as to what experimentation or ancillary analysis is needed for model development or validation, and preliminary assessments regarding prioritization of specific models.

3. MOLTEN SALT REACTOR DESIGN

The molten salt reactors considered in this study are being designed for applications including electricity generation, industrial process heat, and reducing the burden of nuclear waste for future generations by vendors who expect to submit these designs to the NRC for licensing in the near future. The thermal spectrum liquid fuel reactors use a fluoride salt and some employ on-line removal of fission products and possibly actinides. Some have unique ways of adding fissile and fertile material. Fast spectrum liquid fuel reactors are more likely to use chloride salts because of their higher atomic weight and reduced moderating capacity. However, intermediate and fast spectrum designs that use fluoride salts do exist.

[a] Panel members are given in the Appendix.

The four thermal spectrum designs used by the panel collectively as a generic design are the LFTR (by Flibe Energy [8]), ThorCon (by Martingale [9]), IMSR (by Terrestrial Energy [10]) and TAP (by Transatomic Power [11]. For these reactors the very limited available design information is summarized in [5]. For fast spectrum reactors there is even less information available but several concepts are discussed in [5] including two chloride salt designs of interest in the U.S. [12, 13].

4. SIMULATION SCENARIOS

The events that need to be simulated include normal operation, anticipated operational occurrences, design-basis events, and some beyond design-basis events. Since molten salt reactor designs are at the pre-conceptual level, specific design-basis events have not yet been defined. Thus, this study focused on normal operation and a few generic "licensing-basis events." Licensing-basis events are generally initiated by reactivity additions or power-cooling mismatches, the latter either due to a loss of cooling capability or a loss of coolant. Events are simulated to assure that certain acceptance criteria are not exceeded. For liquid fuel reactors acceptance criteria might relate to the maximum temperature for structural materials. The minimum temperature of the molten salt would also be important because the freezing of salt can cause problems such as localized flow blockages.

To date there has not been a comprehensive selection and evaluation of licensing-basis events for molten salt reactor designs. There are no established General Design Criteria (GDC) or a Standard Review Plan specific to molten salt reactors. Indeed, there is not yet a consensus as to what the approach should be to define such events. The discussions in this section are on an ad hoc basis using the best information available in order to identify simulation requirements. They are not meant to define the licensing-basis events that eventually must be analyzed as part of the licensing process.

4.1 Normal Operation

Normal operation is simulated with neutronic and thermal-fluid models to assure that the reactor can be brought to a stable power level with the projected composition of the core and that thermal limits are not exceeded and that reactivity can be controlled. The latter means that shutdown margin, reactivity insertion and withdrawal rates from control elements, and feedback mechanisms (e.g., temperature reactivity feedback) are all acceptable. Normal operation also sets the initial conditions for most licensing-basis events and is the basis for determining the fluence on structures. The assessment of fluence is complex for liquid-fuel MSRs where the source of neutrons and gammas circulates in the primary system.

Ancillary fuel management calculations are needed for any power reactor to determine changes in composition due to irradiation. However, in a liquid-fuel MSR, composition changes can also occur because of the chemistry of the system and because of the deliberate removal of gaseous fission products and possibly certain actinides, and the necessary replenishment of actinides. The systems controlling composition are also important in understanding certain transient/accident events. Hence, simulation tools will be needed to track composition with time and as a function of location within the reactor system and containment structure. The degree to which this tracking is necessary will depend on the particular design.

4.2 Reactivity Events

An unwanted increase in reactivity could be the result of the addition of too much fissile material or the inadvertent withdrawal of control elements. This would cause the power, and simultaneously the temperature of the fluid, to increase. It might also change the spatial power distribution. Negative temperature feedback may control the outcome and/or operators can take corrective actions. Otherwise, reactor trip would be necessary and occur based on either a power or temperature (or possibly, pressure) limiting safety system setting. Corrective actions that the operator might take include the insertion of operable control elements, changes to the fuel processing system, or drainage of the fuel out of the system.

An increase in reactivity could also be the result of a pump trip which causes accumulation of fuel and fission products in the core, including delayed neutron precursors. If more delayed neutron precursors remain in the core, instead of being swept out of the core, this would add reactivity.

A slow increase in reactivity that is unique to reactors with a separate fertile blanket is the loss of the salt from that blanket. One that is unique for reactors with moving moderator rods is the uncontrolled movement of those rods. These events would result in consequences similar to those described above. The loss of salt in the blanket could also be compensated for in a design having a floating control rod in the blanket salt that would add negative reactivity as it moved further into the core while the blanket salt level was dropping.

A rapid increase in reactivity could be caused by the collapse of a significant gas bubble. However, a large bubble would only be possible if there was significant coalescence of dissolved gas. Rapid rates of reactivity insertion in general are unlikely due to the design of the control rod system or the fissile material makeup system. Since MSRs operate at close to atmospheric pressure and control elements enter from above the core, there is no possibility of a control rod ejection or drop (out of core) that could add reactivity quickly (events that are applicable to light water reactors). Nevertheless, it should be noted that even slow additions of reactivity, if unprotected by negative feedback, could potentially lead to energetic excursions.

The opposite scenario is the decrease in reactivity either due to the inadvertent movement of a control rod or bank or the malfunction of the fuel processing system, or the speed-up of a pump, or an injection of secondary system salt through a break in a heat exchanger tube. These have to be analyzed, in particular if there are compensating systems that at the same time may be increasing reactivity.

Because liquid-fuel MSRs have fundamental differences from solid-fuel reactors, a variety of novel scenarios will have to be considered for which there is no precedent for regulatory review. For example, a scenario [8] that is unique to an MSR with a separate circuit for the fertile material is the introduction of negative reactivity due to material control failure in the fuel processing systems. Although this would appear to be a fault that would result in shutdown of the reactor, the associated decrease in temperature could be compensated by a reduction in the blanket salt level in the central control channel—a change that adds reactivity to the core. Thus, in the design of the control system and in the identification of setpoints for activating reactor trip or other actions, consideration must be given to a spectrum of new events.

4.3 Increase/Decrease of Temperature

The unexpected increase or decrease in heat removal from the primary heat exchanger could be caused by numerous initiating events. Faults in the secondary and tertiary systems were only considered through their effect on heat removal by the primary heat exchanger. A decrease in heat removal from the primary system would increase reactivity and the ensuing increase in power would depend on the thermal-hydraulic response of the primary system as well as the response of the plant control system. Too large a decrease could lead to freezing of the salt and the problems that might cause.

A decrease in primary system heat removal would be similar to the increase in temperature due to the failure of one or more pumps in the primary system. In events like this, the core would either come to a new equilibrium power level due to negative reactivity feedback or a reactor trip would occur.

5. IMPORTANT PHENOMENA FOR THERMAL SPECTRUM MSRS

5.1 Figures-of-Merit

The panel generated tables [5] of neutronics phenomena and the potential impacts of uncertainties in the modeling of these phenomena on figures-of-merit during steady state operation. The panel then considered how these assessments of uncertainty would be modified for the analysis of generalized transients characteristic of potential licensing basis events. The tables summarize the state of knowledge of potentially important phenomena affecting reactivity and transient response.

Before generating these tables as part of the pre-PIRT process outlined in Section 2, the panel chose the FoMs in Table I. These FoMs are intended to reflect the importance and impact of specific phenomena. FoM1, reactivity, is an analog for prediction of criticality and also implies accurate prediction of both static and dynamic reactivity during normal operation and transients. This FoM includes special emphasis on the fact that the delayed neutron fraction in the core is directly tied to the motion of delayed neutron precursors and therefore, the flow rate and precursor concentration throughout the primary loop.

FoM2, power distribution and peak power, can be related to design margins for localized peak power limits. These limits must ensure compliance with the key aspects of the applicable GDC related to acceptable fuel design limits that may exist in the future for MSRs. In an MSR, fuel performance and fuel safety include adequate retention of actinides, fission products, and transmutation products within the salt. This FoM envelopes both fission density (cumulative) and fission rate density (instantaneous), and also includes direct energy deposition from neutrons and gamma rays throughout moderator, reflector, and core structure components.

Table I Figures-of-Merit for Thermal Spectrum MSR Neutronics

Figure-of-Merit	Definition
FoM1: Reactivity	Net reactivity and control element reactivity.
FoM2: Power Distribution and Peak Power	Total power and power distribution generated from fission in the salt. This includes neutron and gamma heating in moderator, reflector and structural components.
FoM3: Kinetics Parameters	Reactivity coefficients, delayed neutron parameters, and neutron generation time.
FoM4: Fluence	Neutrons per square centimeter per unit energy.
FoM5: Primary System Gases	Production, removal, and replacement of fission product gases, transmutation product gases, cover gas, and other gases throughout the system.

FoM3, kinetics parameters, includes reactivity coefficients, delayed neutron parameters, and neutron generation time. These parameters will dictate the transient and accident response of the reactor core and primary loop. In addition, these parameters ensure compliance with the requirement that in the power operating range the net effect of the prompt inherent nuclear feedback should compensate for a rapid increase in reactivity. It is noted that FoM3, like FoM1, is related to the motion of delayed neutron precursors throughout the loop.

FoM4, neutron fluence, is directly related to material performance limits. The application of molten salts in advanced nuclear reactor designs requires exposing these salts and associated reactor core materials to extreme conditions. The high neutron flux in the core will generate fission and transmutation products directly in the salt, and these will form a variety of potentially corrosive chemical species. The radiation fields in the core and the chemical species in contact with the core materials will define material performance limits. In particular, core structure and reflector materials that are directly exposed to neutron flux may limit the lifetime of the core, and may lead to failure of components if limits are exceeded. In addition, this FoM is important for potential radiolysis effects in some salts. Experience with the molten salt reactor experiment (MSRE) carried out at Oak Ridge National Laboratory [14], indicates that these effects are minimal, but they are not fully understood for some salts. This also includes the neutron flux-energy spectrum, which impacts the material damage rate.

FoM5, primary system gases and tritium production, refers to the production, removal, and replacement of fission product gases, cover gas, and other gases throughout the system. The formation of fission gas bubbles in the coolant is a potentially important neutronic phenomenon, because these gas bubbles may enter the core and act to poison the fission chain reaction. Additionally, the tracking of tritium throughout the reactor core and structural materials, primary loop, and secondary loop is vital to limit the radiological source term to the public.

The neutronic phenomena considered were listed in a table [5] according to two categories: basic nuclear data and material composition. Basic nuclear data includes the underlying nuclear data libraries, for example ENDF/B-VII.1, that underpin a neutronic model of an MSR. Material composition refers to the accurate modeling of the composition of materials in the core, and throughout the primary loop, including fission and transmutation products. The following summarizes the important points about the phenomena in that table.

5.2 Basic Nuclear Data

^{6}Li Balance: The panel identified basic data sets related to ^{6}Li as impactful. The importance of this isotope in a FLiBe coolant depends on the extent to which it is present as some designs will enrich the lithium in ^{7}Li. The data includes the ^{6}Li neutron capture cross sections, and specifically the (n,t) cross section, which is important for the tritium source term. ^{6}Li has a large absorption cross-section but would be distributed uniformly and have a low impact on power distribution. These phenomena (cross sections) directly impact FoM5 and the tritium source term. The ^{6}Li(n,t)^{4}He cross section and ^{9}Be(n,α)^{6}Li cross sections are both well known. These reactions happen on time scales that are not important for reactor transients. However, the underlying phenomena are important for defining initial conditions for transient events, especially those where tritium release from graphite might be important.

Neutron Moderation and Thermalization by Fuel Salt: The data sets governing moderation and thermalization by the fuel salt will directly impact FoM1 albeit in a relatively small way. The scattering cross sections for F and Li have a low contribution to overall eigenvalue uncertainty and low sensitivity in thermal spectrum MSRs [15]. For thermalization, S(α,β) libraries for F, Li, and Be in FLiBe have been developed and are undergoing testing [16].

Neutron Moderation and Thermalization by Carbon: Moderation and thermalization of neutrons in graphite will have major effects on reactivity (FoM1) and power distribution (FoM2). There is a significant amount of carbon in some designs. These effects are well understood, and can leverage recent insights from the High Temperature Gas Cooled Reactor research and development activities.

Neutron Moderation and Thermalization by Zirconium Hydride: For those designs which utilize ZrH moderator (e.g., TAP [11]), this will have major effects on reactivity (FoM1) and power distribution (FoM2). These effects are reasonably well understood, and can experience from TRIGA reactors should be useful.

Neutron Absorption in Fuel Salt: The corresponding data sets for the initial composition and the composition with fission products and new actinides impacts all the FoMs. These data are generally well-known, the exception being for minor actinides.

Neutron Absorption by Carbon: The absorption cross-section was changed between ENDF/B-VII.0 and ENDF/B-VII.1, as shown in [5]. This can cause differences in excess of 1% in multiplication factor. Although there are differences in the evaluation of the absorption cross-section, indications from the Very High Temperature Reactor Critical (VHTRC) experiments are that the ENDF/B-VII.1 evaluation is a significant improvement over previous evaluations [17]. Some MSR designs have large quantities of carbon. These designs can leverage recent insights from the High Temperature Gas Cooled Reactor research and development activities. The ENDF/B-VII.1 library shows much better agreement with HTGR benchmark experiments, and is preferred for use.

Neutron Production from Beryllium and Fluorine: This includes neutron production in beryllium from (γ,n), (α,n) and (n,2n) reactions. These data may be important for transient analysis where delayed gammas become more important than for steady state. Current computational models do not account for photoneutrons or other neutron production reactions. There are large uncertainties, and potentially significant impacts. Overall, the effect of photoneutrons from Be on the transient behavior of the MSRE was small [18], but the FLiBe salt constituted less than 20% of the volume fraction of the active core. Additionally, it is notable that photoneutrons did have a significant impact on long-term decay power in the MSRE after operation [19]. Recent estimates for the Chinese FHR test reactor indicate about 4 pcm of impact from beryllium photoneutrons [20]. Similar uncertainties exist due to (α,n) reactions in fluorine, but the impact of these reactions is expected to be smaller than the impact of the reactions in beryllium. Calculations should be performed to resolve the uncertainties in data for Be.

Absorption in Control Rod Materials and Fuel Displacement: Absorption in control rod materials, if present in a particular design, is a function of temperature and neutron spectrum. This is very important for FoM1 and FoM2. Reactivity control through the displacement of fuel is a design dependent feature. If this feature is present in the design, the impact on FoM1 and FoM 2 is significant. In either case, measurements would be made to confirm the calculated control element worth.

Neutron Precursor Decay Constants and Fission Yields: These phenomena relate to the production of delayed neutrons in the reactor core and throughout the primary loop—a unique feature of a liquid-fuel reactor. Tracking delayed neutrons and delayed neutron precursors is vital to FoM3. Traditional methods or simplified approaches (e.g. one-dimensional approximations for flow through the primary loop) may or may not be sufficient for calculation of delayed neutron precursor behavior. This is dependent on the reactor design, and is absolutely necessary for simulation of transients, especially long-term transients.

5.3 Material Composition Phenomena

Carbon Density Due to Dimensional Change: Changes in the density of carbonaceous components due to dimensional change, include shrinking at low displacements-per-atom, and swelling at high displacements-per-atom. These dimensional changes effectively divert molten salt fuel outside of the core. Material behavior is outside the scope of the pre-PIRT, and the dimensional change of carbon-based components are not expected to directly impact specific transients for thermal MSRs. Nevertheless, this effect would primarily impact FoM1 and FoM2.

Depletion of Control Rods: This involves the in-core residence time and depletion chains for control materials. In general, liquid fueled reactors would be operated with very low excess reactivity, due to the potential for online refueling. The importance of this phenomenon is design dependent, and not important unless the design uses control rod insertion for reactivity control. For those designs that employ frequent control rod insertion, this may impact shutdown margin and the progression of unprotected transient over-power.

Operational History Effects: This refers to the impact on depletion due to the presence of control rods or other spectrum changing asymmetries within the core, including power operation history; removal rates of fission products, transmutation products, and actinides; and replenishment rates of the salt. Additionally, changes in salt chemistry may impact the retained constituents of the salt, and this could also have history effects. Operational history effects are the result of core average spectrum as a function of time. These effects may be different in two-fluid MSR designs. A special set of chemistry modeling and simulation tools must be developed and coupled to traditional neutronic and thermal hydraulic tools to determine operational history effects.

Isotopes to Track: This is the identification of isotopes to track in depletion simulations, and is closely coupled to the operational history effects. The design and operation of isotope control systems will directly impact FoM1-FoM3. One key outcome of this study is that a separate tool is needed to track MSR chemistry, composition, and isotopes. It is a design-dependent issue as some reactors will also have fuel-processing systems as an integral part of the plant. Consideration must be given to removal of fission products (passive or active), online feed and/or removal of actinides, and continuous or batch discharge of fission products and other material. The chemistry tool must accurately model the thermodynamics of salt phase behavior, fission product solubility, corrosion, and gas transport.

6. IMPORTANT PHENOMENA FOR FAST SPECTRUM MSRS

6.1 Figures-of-Merit

For fast spectrum liquid-fueled MSRs, the panel chose the same FoMs as used for thermal spectrum reactors (see Table I) with the exception for FoM5 where the importance of tritium production is significantly diminished for chloride salt systems. However, for fast spectrum fluoride salts with significant quantities of lithium, the tritium source term will still exist. The important phenomena were again listed in a table {5] with their impact and a path forward. The following summarizes the results.

6.2 Basic Nuclear Data

Cross Sections for Sulfur Production from Chlorine: For fast spectrum MSRs that use chloride salts, chlorine transmutation can result in sulfur production. This may enhance corrosion in the reactor, and requires adequate tracking of chlorine inventories and modeling of salt chemistry conditions.

Neutron Scattering by Fuel Salt: This has a small impact on FoM1, and although scattering behavior at fast energies is well understood, nuclear data uncertainties may exist.

Neutron Absorption in Fuel Salt and Constituents: This includes absorption in the fuel salt, actinides, fission products, and transmutation products. This is defined by the neutron flux and the absorption cross-sections for the fission products and constituents of the fuel salt. As an example, absorption in ^{35}Cl is particularly important. This will impact all FoMs, although fission product poisons and other thermal absorbers will have much less significant impact in a fast spectrum. These effects are generally well known, although nuclear data uncertainties exist. Absorption in actinides will impact breeding ratio and reactivity coefficients, including FoM1 and FoM3. Cross section data for minor actinide isotopes has a high uncertainty, but the overall impact may be low. The delayed neutron fraction, which is already small, will be further reduced by the presence of transuranic actinides.

Absorption in Control Rod Materials and Fuel Displacement: There are no special or unique considerations for fast MSRs relative to thermal MSRs.

Neutron Precursor Decay Constants and Fission Yields: There are no special or unique considerations for fast MSRs relative to thermal MSRs.

Reactor Reflector and Shield Cross Sections: The absorption and scattering cross sections for the reflector and shield elements take on an enhanced importance in fast spectrum systems because leakage reactivity is higher, and may play an important role in fast inherent feedback. These data are design dependent, in that they depend on materials comprising the reflector and shield and the neutron leakage spectrum from the reactor core. The cross sections are generally well known.

6.3 Material Composition Phenomena

The need for understanding material composition is important and many of the considerations for thermal spectrum MSRs are valid. For some molten salt fuel compositions and mixtures, there is limited knowledge about phase diagrams and potential radiolysis. Relatively sparse data exist for radiation and thermal stability of some potential salts, especially chloride salts. Phase diagrams of some salts are relatively unknown in the presence of fission products, transmutation products, and impurities. Although the MSRE experience indicated high radiation stability for that particular fuel salt mixture (LiF-BeF_2-ZrF_4-UF_4), the operating neutron spectrum was thermal and the displacements per atom rate was low. Fundamental thermodynamic data, such as Gibbs free energies and interatomic potentials, are needed to develop these phase diagrams.

Reactor Reflector and Shield Material Density: This refers to changes in the density of the reflector and shield components due to thermal expansion. These dimensional changes may change the volume of molten salt in different locations or change leakage from the core. Material properties must be provided by the applicant or determined experimentally with appropriate qualification. These materials are currently unknown.

Fuel Salt Density: This refers to the density of the fuel salt, including any gas bubbles present in the mixture, as a function of temperature and gas presence. This will impact FoM1-FoM3 and is important for providing fast inherent negative feedback. The feedback mechanisms and effect of gas bubbles on reactivity must be determined. As a feedback effect, this is highly important for reactor transients or accidents.

Operational History Effects: There are no special or unique considerations for fast MSRs relative to thermal MSRs.

7. SUMMARY AND CONCLUSIONS

The NRC is working toward the goal of being able to do confirmatory calculations when applications come from vendors of liquid-fuel MSRs. A first step in having the simulation capability is identifying the physical processes that need to be modeled so that existing codes and new modeling can be implemented. A pre-PIRT was carried out by having a group of subject matter experts define the important phenomena for neutronics modeling, their importance, and the current state-of-the-art. They also helped define what the path forward might be for important phenomena.

The panel identified basic nuclear data and material composition challenges that impact simulation of neutronics for steady state and transients in thermal spectrum liquid fuel MSRs. The basic data needs that are most important are for components of the salt that would be used. The presence of "light" elements like F, Li, Be impacts neutron moderation and thermalization. The potential for significant tritium production from Li (especially from ^{6}Li) and neutron production from F and Be (e.g., from (γ ,n) and (n,2n) reactions) also make data for these elements important. The reactor physics for these nuclides (and other nuclides that are part of the fuel and structure) are relatively well known or currently being studied. Nevertheless, there will be a need for more confirmatory analysis in the future.

A unique reactor physics challenge relates to delayed neutron precursors. The major challenge is not the physics data (precursor fractions and decay constants) but rather the physical location of delayed neutron precursors as they circulate in the system. This will be a challenge although it has been demonstrated that the impact of the movement of precursors may be able to be conservatively bounded. This is because in support of the MSRE a relatively simple model was used to show that the MSRE dynamics could be so modeled [21]. That model predicted that the reactor was stable and controllable over its power range and an extensive experimental program validated that model [22] for that particular reactor.

Material composition is very important for determining neutronics behavior (and source terms for accident analysis) in a liquid fuel reactor and challenging because of its dynamic nature—especially when there is fuel processing taking place as the reactor operates. Fission products and actinides are being produced in the reactor as are other transmutation products. Chemical interactions in the salt add another complexity in determining composition (and is also important for corrosion issues). Corrosion, particle agglomeration, filtering, plate-out of insoluble components all impact composition. Depending on design, there may be removal of certain fission products, actinides, or gaseous components. The tracking of material composition then must be a part of any neutronics simulation and this involves not only reactor physics but also chemistry and material transport.

The basic data needs for fast spectrum MSRs are different from those for thermal spectrum reactors as the materials used for the fuel salt and possibly the structures will be different. Uncertainties exist currently by virtue of not knowing what materials will actually be used. One certainty is that if a chlorine salt is used, the isotope ^{35}Cl will be of particular interest because of its large cross section.

In conclusion, this study has identified key neutronics phenomena that are vital for the modeling and simulation of MSRs, with liquid-fuel. The large number of system designs means that there is wide variation in the potential predictive modeling needs. The phenomena identified in this paper are design independent, because none of the designs have progressed to the needed level of maturity to conduct a full PIRT—an activity that will be necessary at a later date.

ACKNOWLEDGMENTS

The authors of this report are indebted to all the members of the pre-PIRT panel (whose names are found in the Appendix to this report). Their focused efforts, during a long day of getting their expert input on the subject, were vital to providing the information contained in this paper.

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APPENDIX
MEMBERS OF THE PRE-PIRT PANEL

Stephen Bajorek (Chair)
U.S. Nuclear Regulatory Commission
Washington, DC 20555-0001

David Diamond (Facilitator)
Brookhaven National Laboratory
Upton, NY 11973-5000

Mark Anderson
University of Wisconsin
Madison, Wisconsin 53706

Nicholas Brown
Pennsylvania State University
University Park, PA 16802

Richard Denning
Independent Consultant
Columbus, Ohio 43220

David Holcomb
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831-6170

Nathanael Hudson
U.S. Nuclear Regulatory Commission
Washington, DC 20555-0001

Andrew Ireland (Scribe)
U.S. Nuclear Regulatory Commission
Washington, DC 20555-0001

Joseph Staudenmeier
U.S. Nuclear Regulatory Commission
Washington, DC 20555-0001

Xiaodong Sun
University of Michigan
Ann Arbor, Michigan