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Phenomena Important in Molten Salt Reactor Simulations

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Phenomena Important in Modeling and Simulation of Molten Salt Reactors

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ABSTRACT

The U.S. Nuclear Regulatory Commission (NRC) is preparing for the future licensing of advanced reactors that will be very different from current light water reactors. Part of the NRC preparation strategy is to identify the simulation tools that will be used for confirmatory safety analysis of normal operation and abnormal situations in those reactors. This report advances that strategy for reactors that will use molten salts (MSRs). This includes reactors with the fuel within the salt as well as reactors using solid fuel. Although both types are discussed in this report, the emphasis is on those reactors with liquid fuel because of the perception that solid-fuel MSRs will be significantly easier to simulate. These liquid-fuel reactors include thermal and fast neutron spectrum alternatives. The specific designs discussed in the report are a subset of many designs being considered in the U.S. and elsewhere but they are considered the most likely to submit information to the NRC in the near future.

The objective herein, is to understand the design of proposed molten salt reactors, how they will operate under normal or transient/accident conditions, and what will be the corresponding modeling needs of simulation tools that consider neutronics, heat transfer, fluid dynamics, and material composition changes in the molten salt. These tools will enable the NRC to eventually carry out confirmatory analyses that examine the validity and accuracy of applicant's calculations and help determine the margin of safety in plant design.

The study makes use of the limited amount of experience with such concepts, for example, from the 8 MWt Molten Salt Reactor Experiment at Oak Ridge National Laboratory in the 1950s and 1960s, and recent conceptual design studies. Since the latter studies are so preliminary, the present work focused on the primary system, and did not consider in detail systems for secondary or tertiary heat removal, decay heat removal, and reactor cavity cooling, nor operation of emergency shutdown equipment. This study will facilitate decisions in the future, as to required simulation tool capabilities and what research is necessary before such tools can be successfully used.

The identification of modeling needs for liquid-fuel MSRs was carried out by subject matter experts, using a process frequently used by NRC to elicit information; namely, the Phenomena Identification and Ranking Table (PIRT). However, since that process would normally require knowing specific details about a reactor design and the sequence of events during accidents and since MSR designs are varied and not yet well defined, the process used was considered a "pre-PIRT" and the panel considered what might happen generically if there were changes in reactivity in the core or changes in temperature.

The panel met after reviewing the available information on design details and postulated normal and abnormal operation. They defined phenomena that would need to be modeled and considered the impact/importance of each phenomenon with respect to specific figures-of-merit (e.g., peak power, fluence, flow velocity, temperature). Each figure-of-merit reflects a potential impact on radionuclide release or loss of a barrier to

release. The panel also considered what the path forward might be with respect to being able to model the phenomenon in a simulation code. Subsequent to the pre-PIRT meeting, this report was written to capture the information from the panel and add other relevant material.

The tables of phenomena, their impact and a proposed path forward for filling in the technology gaps were generated separately for neutronics and thermal-hydraulics for thermal spectrum and fast spectrum liquid-fuel reactors. There is already considerable information in the literature on the simulation of solid-fuel MSRs. The tables give a sense of what are the most important phenomena and of those, which ones are the least well understood and hence will require the most effort to be modeled in the future.

The neutronic phenomena are broken into two categories: basic nuclear data, and material composition. The latter is particularly important for liquid-fuel MSRs and is discussed extensively in the report because material inventory and distribution may be continuously changing due to the addition of fissile material, the removal of fission products and/or certain actinides, and chemical interactions and radiolysis possible in the molten salt. The thermal-hydraulic phenomena are broken into categories representing different systems/components: fuel salt, core materials, primary pumps, and primary heat exchanger.

In addition to discussing the specific phenomena in each table, the report considers more generally the issue of inventory control and distribution, and experimental and other research needs and provides a summary of recommendations related to these aspects. It is expected that as an MSR design nears its final stages and is submitted to the NRC for review, a PIRT panel will re-examine the information in this report and will identify what additional work must be done to have the desired simulation capability.

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ACKNOWLEDGEMENTS

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 report. Thanks also to panel member Mark Anderson for contributing to the section on experimental gaps.

ACRONYMS

AHTR	Advanced High Temperature Reactor
ARE	Aircraft Reactor Experiment
ATWS	Anticipated Transient Without SCRAM
CSAU	Code, Scaling, Applicability and Uncertainty
DRACS	Direct Reactor Auxiliary Cooling System
FHR	Fluoride High Temperature Reactor
FoM	Figure-of-Merit
GDC	General Design Criteria
HTGR	High temperature Gas-Cooled Reactor
IMSR	Integral Molten Salt Reactor
LFTR	Liquid Fluoride Thorium Reactor
LOCA	Loss-of-Coolant Accident
LOFC	Loss of Forced Convection
LWR	Light Water Reactor
MCFR	Molten Chloride Fast Reactor
MSFBR	Molten Salt Fast Breeder Reactor
MSR	Molten Salt Reactor
MSRE	Molten Salt Reactor Experiment
NRC	U.S. Nuclear Regulatory Commission
NRO	Office of New Reactors
ORNL	Oak Ridge National Laboratory
PARCS	Purdue Advanced reactor Core Simulator
PB-FHR	Pebble Bed Fluoride High Temperature Reactor
PIRT	Phenomena Identification and Ranking Table
SFR	Sodium-Cooled Fast Reactor
TAP	Transatomic Power Reactor
TRACE	TRAC and RELAP Advanced Computational Engine
TRISO	Tristructural Isotropic Fuel Particle
VHTRC	Very High Temperature Reactor Critical

1 INTRODUCTION

1.1 Background

The Office of New Reactors (NRO) of the U.S. Nuclear Regulatory Commission (NRC) is preparing for the future licensing of advanced reactors that 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 [1-1][a] 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 [1-2] 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." Ultimately, the consequences of reactor accidents are assessed with regard to the magnitude of radiological (or hazardous material) exposure to members of the public. Although it will be necessary for the NRC to develop tools for assessing the release and transport of radioactive material in accidents, the immediate priority is to identify a set of computational tools that can 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. It is vital to understand and be able to predict behavior during normal operation, anticipated operational occurrences, transient events, and accidents and the physical phenomena that dominate those events.

As part of the NRC evaluation of a new design, confirmatory safety analyses are performed in order 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. This may be particularly important with non-LWR designs where there is much less regulatory experience and much less computational experience relative to LWR designs. The calculations performed by the NRC as part of a confirmatory analysis do not represent licensing basis for a design. This is the responsibility of the applicant, who may choose to perform conservative calculations with bounding assumptions. The NRC calculations, because they are concerned with safety margin, are generally performed with realistic assumptions and models that are intended to represent the actual behavior of the plant.

For liquid-fuel molten salt reactors (MSRs) with on-line reprocessing, there are greater uncertainties about safeguarding special nuclear material that could be used in the production of nuclear weapons, than for LWRs. The neutronics tools developed to characterize the changing inventory of radionuclides that establish the initial conditions for safety analyses will also be useful in the performance of safeguards analysis.

[a] References are provided at the end of every chapter.

Before one can select or develop the simulation codes, it is necessary to first understand the scenarios that will need to be analyzed. This requires understanding the design of advanced reactors and then understanding normal operation and the potential upsets that may occur. The next step is to understand what physical processes must be modeled by the computer codes. It is at that point that NRC can survey the existing codes to see which might be optimal, with one of the criteria being that it requires the least amount of resources. “The emphasis in the [NRC] staff’s approach is to leverage, to the maximum extent practical, collaboration and cooperation with the domestic and international community interested in non-LWRs with the goal of establishing a set of tools and data that are commonly understood and accepted.” [1-1, 1-2]

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 where developing simulation tools might be most challenging. This subject includes reactors with fast or thermal spectra and with solid fuel or fuel dissolved in the salt.

1.2 Objective

The objective of this work is to start the process outlined in Strategy 2 for molten salt reactors, that is, to understand the modeling needs of simulation codes. Phenomena identified as important in this report will be used in the selection and development of computer codes for MSR analysis. Computer codes must be able to simulate these processes, unless a suitable approximation or bounding assumption can be applied. Thus, phenomena identified as important will be used to make a judgement on code applicability to an MSR. Due to the preliminary nature of the information available on various MSR designs, the focus for the project is the primary system and not secondary or tertiary heat transport systems or auxiliary systems for residual heat removal. The accident phenomena of interest include events leading up to the potential failure of the system boundaries. For solid-fuel molten salt reactors, this would include events resulting in cladding failure, as well as primary system failure. In liquid-fuel reactors, the failure of the primary system boundary, including the potential melting of a freeze plug if present, represents the potential for the release of radionuclides. The focus herein is on liquid-fuel reactors as there is much more information already available in the literature on modeling needs for solid-fuel reactors (e.g., [1-3, 1-4, 1-5]).

The modeling of radionuclide release and transport is not considered in this pre-PIRT. Because the retention mechanisms for fission products are so different from those in LWRs, this will need to be an area of special focus in the future. This is particularly true for tritium generation, transport and release for concepts using lithium or beryllium-containing salts. Accidents associated with fuel processing that might be an integral part of a liquid-fuel MSR plant are also 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 the NRC's TRACE and PARCS codes as well as several of the U.S. Department of Energy's codes for application to MSRs.

1.3 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) [1-6]. 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 also 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. Although there is sufficient information for some non-LWR designs to undertake a full PIRT, 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. Nevertheless, a PIRT-like activity, referred to as a "pre-PIRT" in this report, has value 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. Chapter 2 describes the reactors of interest. For the liquid-fuel fluoride salt reactors there is very little information available on new designs (although considerable information is available from the molten salt reactor experiment that ran at Oak Ridge National Laboratory for several years starting in 1965 [1-7]). For chloride salt fast spectrum reactors there is even less information available. Fixed fuel reactors using fluoride salts have more information available and are also discussed.

The pre-PIRT panel[b] first considered normal operating conditions, which typically establish the initial conditions for accident scenarios. Even steady-state modeling is a challenge. They then considered generic transient conditions, such as reactivity insertion accidents, flow coast-down accidents, and loss of primary system heat

[b] Panel members are listed in Appendix A.

removal rather than a set of design-basis and beyond design-basis accidents specific to a particular design. Chapter 3 provides a discussion of the types of licensing-basis events that may be simulated with the computer tools of interest.

Chapter 4 discusses the physical processes that must be modeled in order 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 safety related concern of the NRC is generally 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. In the pre-PIRT process, the panel first addressed the phenomena associated with steady-state operation of the plant. Consideration was then given to how the assessment for steady-state operation should be modified to address the ability to analyze transient/accident conditions.

The panel also provided remarks on 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 this work.

This report contains the background information enhanced by the discussions of the panel and roughly prioritizes the neutronic and thermal-fluid (aka thermal-hydraulic) phenomena according to research needs for future simulation tool development. Phenomena that are of high importance and where the knowledge level is lowest have the greatest needs and will be where the focus is in the future; conversely those with low importance or are fully understood will not require attention going forward.

Chapter 5 provides a summary of the findings of this study and recommendations for future work.

1.4 References

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1-6 G. E. Wilson and B. E. Boyack, “The Role of the PIRT Process in Experiments, Code Development, and Code Applications Associated with Reactor Safety Analysis,” *Nuclear Engineering and Design, 186*, pp 23-27, 1998.

1-7 “An Evaluation of the Molten Salt Breeder Reactor,” WASH-1222, U.S. Atomic Energy Commission, September 1972.

2 DESCRIPTION OF MOLTEN SALT REACTORS

2.1 General Design Features

The molten salt reactors that are under consideration are being designed for generating electricity and process heat by vendors who expect to submit these designs to the NRC for licensing in the near future. The reactors use either solid fuel or liquid fuel, that is, fuel mixed with the molten salt. In general, the solid-fuel reactors are fluoride salt cooled high temperature reactors and are referred to as FHRs. They are expected to use TRISO fuel particles within a graphite matrix; a similar configuration to what has been proposed for high temperature gas-cooled reactors (HTGRs). 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.

In the following sections, the design features that are known for these reactors are explained. The emphasis is on those designs under development by specific vendors, although it is recognized that some of these designs are also being supported by work at universities and national laboratories in this country. It is also recognized that there are alternative designs being worked on at research centers in the U.S. and around the globe. The work being done on those other designs, not emphasized herein, is very important and is discussed in this report when applicable. That work also helps to inform how the pre-PIRT panel contributes to the problem at hand. Each of the concepts reviewed is at a very early stage of development, and the specific information about the designs is subject to change. The purpose of this chapter is to provide information on the potential range of characteristics of MSR designs.

2.2 Thermal Liquid-Fuel Molten Salt Reactors

Four MSR designs under development with liquid fuel using a fluoride salt are listed in Table 2-1 with key parameters to help understand basic design and how accident scenarios might progress. The parameters and design features listed in the table come from a variety of sources (see references in table). Each potential vendor has a website (listed in Table 2-1) but the extent of useful information in those websites and corresponding references differs from one design to the next. These designs are all very preliminary, some not even "pre-conceptual," and hence, more important than the specifics of the design are the common features and phenomena that must be modeled in any future accident simulations. All of these designs are expected to evolve and change.

The first three rows in Table 2-1 are the vendor name, reactor name and proposed power level, the latter being a first estimate. Terrestrial Energy has also proposed an 80 MWt prototype and Transatomic Power has proposed a 20 MWt prototype. However, for the purposes of this study, higher power levels are considered.

Table 2-1 Fluoride Salt (Liquid Fuel) Reactor Concepts

Organization	Flibe Energy	Martingale	Terrestrial Energy	Transatomic Power
Reactor Name	**LFTR**	**ThorCon**	**IMSR**	**TAP**
Power	600 MWt	557 MWt	300 or 600 MWt	1250 MWt
Reactor Core				
Fuel Salt	LiF-BeF_2 -(Th/U)F_4	NaF-BeF_2-(Th/U)F_4	NaF-RbF-UF_4 (or LiF-BeF_2-UF_4)	LiF-(U/Pu/La)F_4 5% enriched U SNF in later editions No Be
Max Fuel Temperature	653°C	704°C	-	650°C
Moderator	Graphite tubes	Graphite plates in hexagonal assemblies	Graphite	Moveable ZrH rods (clad) to obtain spectral shift
Spectrum	Thermal	Thermal	Thermal	Thermal-epithermal
Reflector	Blanket and core salts are separate Blanket heat transfer may be in vessel	Graphite radial reflector	-	Moveable ZrH moderator
Fuel Processing				
Gaseous FP Removal	Assisted	Assisted	Off gases in space above	Assisted
Other FP Removal	Bismuth FP extraction	Offsite FP removal every 8 years	Offsite FP removal Tank removed every 7 years	Offsite bismuth FP extraction Plate out on nickel filter
Other Processing	Pa/^{233}U separation (from Th)	Offsite uranium separation	_	_
Safety Features				
Reactivity Control	Shutdown rod Central regulating control rod Floating blanket control rods	Central control/shutdown rods	Flow-driven shutdown rod Meltable can with poison as secondary shutdown	Shutdown rod and movement of ZrH rods

Organization	Flibe Energy	Martingale	Terrestrial Energy	Transatomic Power
Miscellaneous	Freeze valve/drain tank	Freeze valve/drain tank Sealed primary loop Continuous passive decay heat removal	Water cooling jacket surrounds buffer salt zone outside core for decay heat removal No drain tank	Freeze valve/drain tank Passive air cooling
Other Design Features				
Secondary Coolant Salt	$NaBF_4$ - NaF	NaF - BeF_2	KF-ZrF	LiF - KF – NaF (FLiNaK)
Vessel and Primary Piping Materials	Hastelloy N	SS316Ti	Hastelloy N -	SS316 + Hastelloy N
Website	flibe-energy.com	thorconpower.com	terrestrialenergy.com	transatomicpower.com
References	[2-4, 2-7]	[2-5]	[2-6]	[2-2, 2-3]
LFTR – Liquid Fluoride Thorium Reactor *IMSR – Integral Molten Salt Reactor* *TAP – Transatomic Power Reactor*	*MA – Minor actinides* *La – Lanthanides* *FP – Fission product* *SNF – Spent nuclear fuel*			

There are several characteristics under “Reactor Core” in the table. The salt is always a fluoride with different constituents depending on design. When lithium is used, it is assumed it will be fully enriched to ^{7}Li in order to remove ^{6}Li to the extent possible. ^{6}Li is an efficient neutron absorber and undesirable tritium producer. The TAP design chooses to eliminate the presence of beryllium in the salt. This reduces the risk from its chemical toxicity and allows for a higher concentration of uranium relative to a FLiBe salt.

The enrichment of ^{235}U in the uranium is specified as less than 5 weight percent (w/o) for the IMSR but is not known for the other designs. It is expected to be up to 5 w/o to take advantage of current regulations, but possibly up to 20 w/o, the limit allowed for low-enriched uranium. The TAP design considers very low enrichment (down to 1.8 w/o) that is possible in the very thermal spectrum that can be created using the ZrH moderator rods. The LFTR and ThorCon reactors intend to use thorium in order to make the reactors more fuel efficient and the TAP design also uses various actinides and spent fuel to foster burnup of long-life radioisotopes. More information on the use of thorium is found in [2-1].

The core outlet (maximum fuel) temperature is given for three of the designs. The temperatures are expected to exceed 600°C. All design will operate at, or close to, atmospheric pressure.

All four reactor cores have moderating material and in three of the designs the moderator is graphite and the spectrum is thermal. In the TAP design, the moderator consists of small diameter zirconium hydride rods with a corrosion resistant cladding. The latter are moveable so that the core starts a fuel cycle with an epithermal spectrum that becomes increasingly thermal with time as the rods are inserted. The schematic for the TAP design is shown in Figure 2-1 and more information on how the spectrum is used to control reactivity is given in [2-2] and [2-3].

The salt in each of these designs also plays a moderating role because of the presence of low atomic mass elements like lithium and beryllium (and to some extent fluorine). In most designs it is expected that an increase in temperature of the salt will lead to negative reactivity feedback due to the decrease in salt density and the Doppler effect in the ^{238}U present.

The salt flows in an upward direction in each of these cores, passing through the moderator structure that differs by design. For example, the LFTR design uses hollow graphite “logs” which form cylindrical tubes in which the salt flows. Figure 2-2 is a rendering of the LFTR [2-4] showing the flow tubes.

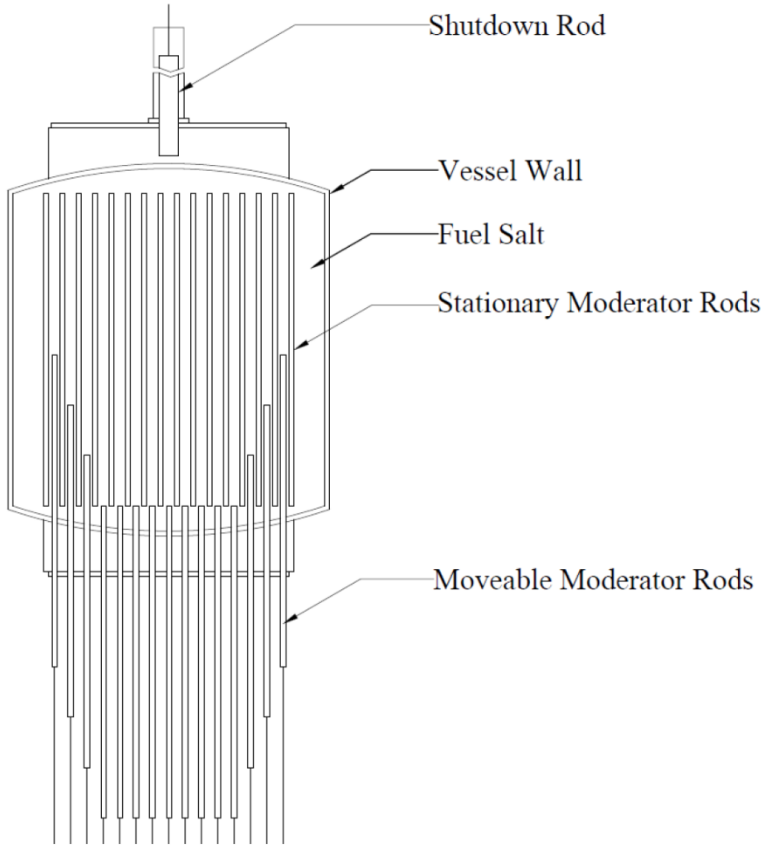

Figure 2-1 TAP Schematic Showing Moveable Moderator Rods [2-2]

Figure 2-2 also shows the distinction between core (blue) and blanket (green) graphite flow channels in the LFTR. The blanket contains thorium salt utilized to generate fissile ^{233}U. It is a separate system with the salt going through a heat exchanger that may be located within the vessel--as opposed to the primary heat exchanger for the core molten salt which is to be located outside the vessel. Note too that the black logs shown at the periphery of the core form a graphite reflector.

The ThorCon design uses hexagonal assemblies with the graphite arranged in plates between which the salt flows. These are shown on the core layout in Figure 2-3 [2-5] which also shows the graphite elements that make up the reflector.

A schematic for one proposal for the IMSR is shown in Figure 2-4 [2-4]. In this design there is a salt buffer between the core and the containment whereas in other designs the space is empty. Although it does not provide any detail on the core geometry, it does show that the primary molten salt remains in the basic reactor vessel with only the secondary coolant moving through piping outside the vessel.

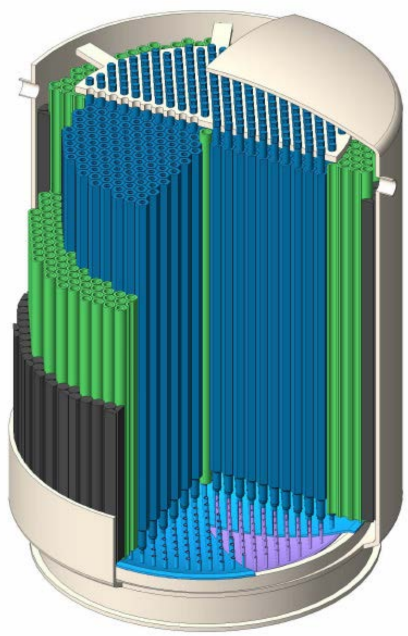

Figure 2-2 LFTR Core [2-6]

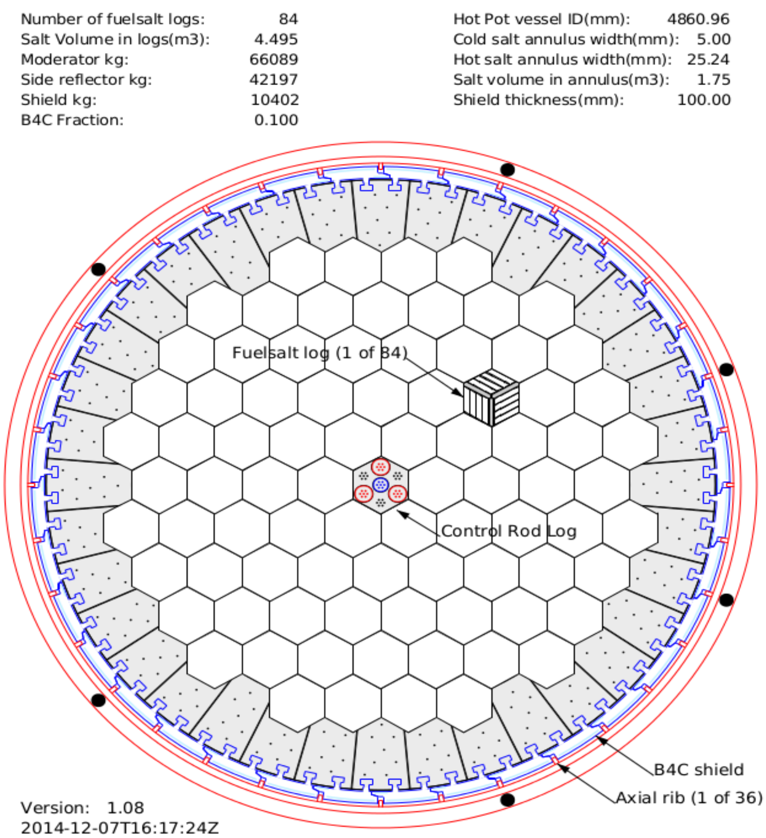

Figure 2-3 ThorCon Core Layout [2-5]

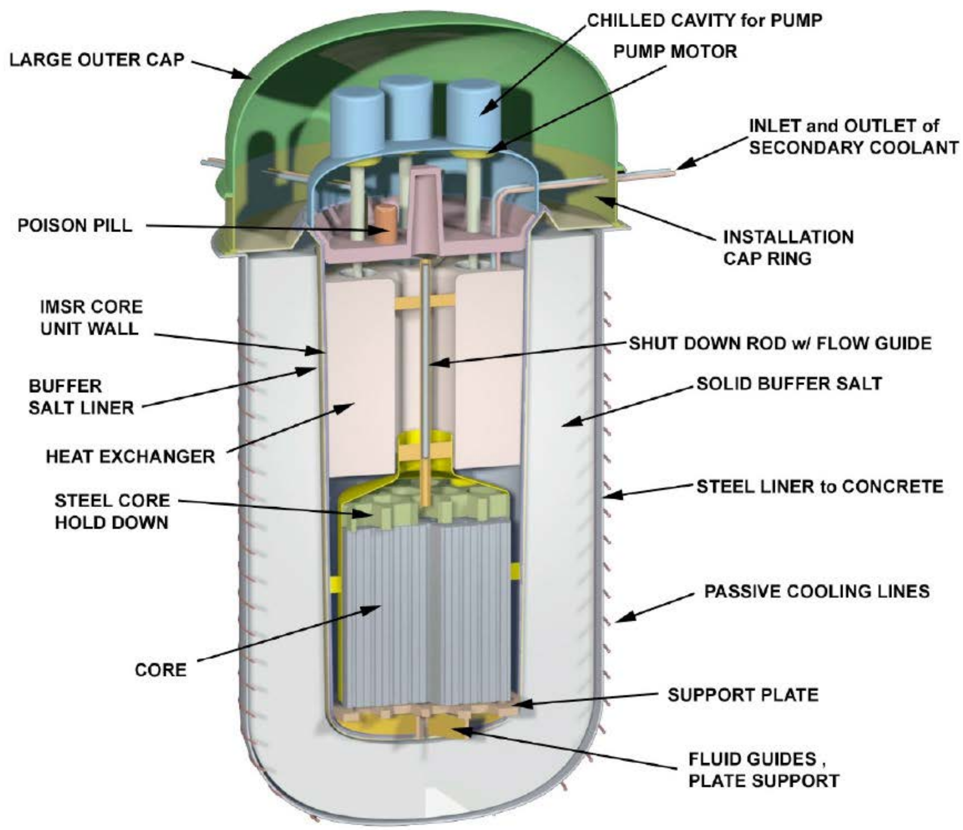

Figure 2-4 IMSR Design [2-4]

The next section in Table 2-1 has information on how the fuel composition may change with time, that is fuel processing. This is important for understanding core (and system) behavior as the removal of fission products and actinides, and the addition of fissile and/or fertile fuel, could change the composition of the core on a continuous basis.

The first feature under safety features in Table 2-1 is reactivity control. This is also an item with few details available. All designs will obviously have shutdown rods. Since a liquid-fuel reactor can operate with little excess reactivity, the reactivity worth of the shutdown rods does not have to be high. Two of the designs (LFTR and IMSR) intend to use floating (or flow-driven) shutdown rods with those for the LFTR located in the blanket. These rods are above the core under normal flow patterns but will fall into the core if flow is interrupted.

As a secondary shutdown system, the IMSR may have a can filled with a (unknown) neutron poison (see “poison pill” in Figure 2-4). The can will melt under scenarios where the molten salt gets above a certain temperature. Although this is useful if there is an anticipated transient without reactor trip, it is not clear why this might also apply when the reactor is shut down but the temperature rises for another reason.

According to [2-6], “An active set of control rods, of a more conventional design, would also be present in the [LFTR] reactor vessel and would [allow] the operator to control the reactivity level of the reactor. These rods, which would comprise a smaller and less potent source of negative reactivity, would be clustered near the center of the core and provide finer control over reactivity levels. Another possibility for these rods would be to replace them with a pneumatic system that [would] hold blanket salt down through gas pressure in a central channel. Through control of gas pressure, the level of blanket salt in these channels might also be controlled. This alternate approach … would have the advantage of being able to "fail open" by releasing gas pressure, allowing blanket salt level to rise in these channels, and thus introducing the desired negative reactivity.”

Minor reactivity changes can be achieved through temperature changes or in the TAP design by moving the ZrH moderator rods.

One safety feature on three of the designs is a drain tank below the vessel with a freeze plug at the entrance. The material for this plug has not been specified, nor are the requirements for a cooling system. Overheating the liquid fuel, or perhaps operator action, would allow the molten salt to flow into a drain tank with geometry that would prevent criticality.

Decay heat removal from either the initial configuration (fuel in the primary system), or with fuel in the drain tank, will be another important part of each design where little is currently known. The IMSR design shown in Figure 2-4 has a solid salt barrier on the outside of the core and this will act as a heat sink in the event that normal heat removal fails.

Two other features are listed in Table 2-1 that are of general interest but only peripherally relevant for the pre-PIRT. These are the proposed molten salts in the secondary circuit and the materials being proposed for key components such as the vessel and piping.

2.3 Molten Salt Fast Reactors

Fast spectrum molten salt reactor concepts have been considered for a number of years, particularly as potential breeder reactors or as actinide burner reactors. In 1956, ORNL described a “fused salt” fast reactor concept consisting of a homogeneous mixture of chloride salts: NaCl, $MgCl_2$, and $Pu(U)Cl_3$ [2-7]. The uranium was in the form of depleted uranium. An external blanket region was used to improve the overall breeding ratio. The core region was internal to a nearly spherical vessel tapered at the bottom and top for inlet and outlet pipe connections. Chloride salts were selected rather than fluoride salts to decrease the amount of spectrum moderation within the core. The thermal power of the design was 700 MWt and with a 37.1% efficiency the electric output was 260 MWe. Continual on-site reprocessing of fuel was assumed. The principal development issues identified were: the corrosive nature of the salt and the development of suitable vessel materials; the large fuel inventory required because of the external fuel hold-up; poor heat transfer properties of the salt; and low specific power density relative to other design concepts under development. A number of different reactor design concepts were under development at the time and sodium fast breeder reactor concepts soon became the focus of the breeder reactor development effort.

When the international Gen-IV initiative was initiated, one of the design concepts selected for development was the molten salt reactor. In addition to the development of thermal spectrum MSR concepts, fast spectrum designs are also under development. The Molten Salt Fast Breeder Reactor (MSFBR) concept developed by the Center for Scientific Research at Grenoble and the French company INOPRO [2-8] involved modifications to the initial Molten Salt Breeder Reactor design, which was a thermal spectrum Th/^{233}U breeder reactor concept with a very low breeding ratio. By removing the graphite moderator in the core region, the concept became a fast spectrum reactor. The MSFBR is a 3000 MWt reactor with three hydraulic loops: the primary system in which the molten fuel salt of actinide fluorides dissolved in LiF circulates, an intermediate heat transfer loop, and a power conversion system. The Li is highly enriched in the isotope ^{7}Li. The concept includes a radial blanket salt of LiF and ThF to increase the breeding ratio. A gas injection system is used to remove gaseous fission products from the molten fuel. Among the design issues addressed in the evolution of the design were the removal of internal structures within the core region to reduce potential problems associated with corrosion and vibration and optimizing the shape of the core cavity.

The REBUS [2-9] reactor design, developed by Electricité de France, has many similarities to the MSFBR but the fuel salt is a mixture of trichlorides of uranium and transuranics dissolved in NaCl. REBUS is a 3700 MWt reactor. It would operate on a uranium-plutonium closed fuel cycle. The assumed vessel wall material is titanium to withstand the corrosive properties of chloride salts. Similar to MSFBR there would be no reactor internals and a radial blanket region to increase the breeding ratio. The primary system vessel is cylindrical.

Preliminary safety analyses for the REBUS design indicate that unprotected loss of flow accidents present a safety challenge because there is both a reduction in heat removal and an increase in reactivity because of the greater residence time of fuel within the core region. In addition, the coefficients of thermal expansion of the chloride salts are not well known. It is likely that a dump tank capability would be provided to enable the salt to be contained in a subcritical, coolable geometry.

There are two groups working on liquid-fuel reactors that would have a fast spectrum that are targeting the U.S. market. From the very limited information publicly available, both are proposing to use chloride salts. It has been proposed to use UCl_3 (and possibly $TRUCl_3$) as the fuel bearing salt and NaCl (and $MgCl_2$) as the carrier salts. Since chlorine is 76% ^{35}Cl which has a significant neutron cross section, the possibility of eliminating the isotope through enrichment has been considered.

One group, led by Southern Company Services has as partners, TerraPower, Electric Power Research Institute, Vanderbilt University and Oak Ridge National Laboratory [2-10]. This group has funding through the Department of Energy and is working on a pre-conceptual design and materials suitability. The very limited public information available indicates that this design will be based on chloride salts.

The other group, Elysium Industries, was founded in 2015 to develop and market the Molten Chloride Fast Reactor (MCFR). It is headquartered in Vancouver, Canada, with offices in the U.S. Little has been published about the design details other than it is a 2500 MWt (1000 MWe) design, would use chloride salts and would use a freeze plug to dump the fuel salt into a cooled, safe-geometry tank in the event of over-temperature conditions [2-11].

2.4 Solid-Fuel Molten Salt Reactors

Solid-fuel molten salt reactors (FHRs) use fluoride salts and operate at relatively high temperatures. They use TRISO particle fuel within a graphite matrix that provides the principal moderation (the salt being the other source of moderation). A TRISO (tristructural-isotropic) fuel particle is a small (one millimeter diameter) sphere comprised of three layers: a uranium core coated with a layer of carbon, a layer of silicon carbide and an outer layer of carbon. Although testing is still underway, the expectation is that the spheres will withstand very high temperature (e.g., 1800°C) without cracking and with very little release of fission products [2-12]. Depending on the core design the TRISO particles are either contained within graphite pebbles or monolithic blocks of graphite. The approach being taken by one potential vendor, Kairos Power [2-13], is to use pebble fuel. The effort is supported by the University of California (UC) at Berkeley. Since little is known directly from Kairos Power, the similar Mark 1 PB-FHR design being developed by UC-Berkeley [2-14] is considered in this pre-PIRT exercise. In addition, the Advanced High Temperature Reactor (AHTR) [2-15, 2-16] is considered for insights into FHR design. The AHTR uses plate fuel to hold the TRISO particles but has similarities to the PB-FHR due to its use of a fluoride salt as coolant. General information on FHR design is also available [2-17].

Figure 2-5 is a diagram of the Mark 1 PB-FHR plant and Table 2-2 lists design parameters for this concept and the AHTR. In the table DRACS refers to the Direct Reactor Auxiliary Cooling System shown in the figure which is used if the normal shutdown cooling system is not functional. Both reactors operate at low pressure and use pool-type reactor vessels.

The fuel pebbles for the PB-FHR are 3.0 cm in diameter with a graphite core, a layer containing 4730 TRISO fuel particles and an outer layer of high density graphite. They are placed in an annular core, bounded by a central graphite moderator and radial graphite reflectors. The pebble bed has a coolant fraction of 40% and is fed from multiple locations at the bottom. The pebbles float in the salt so in practice they slowly move toward the top where they are removed and considered for reentry or removal.

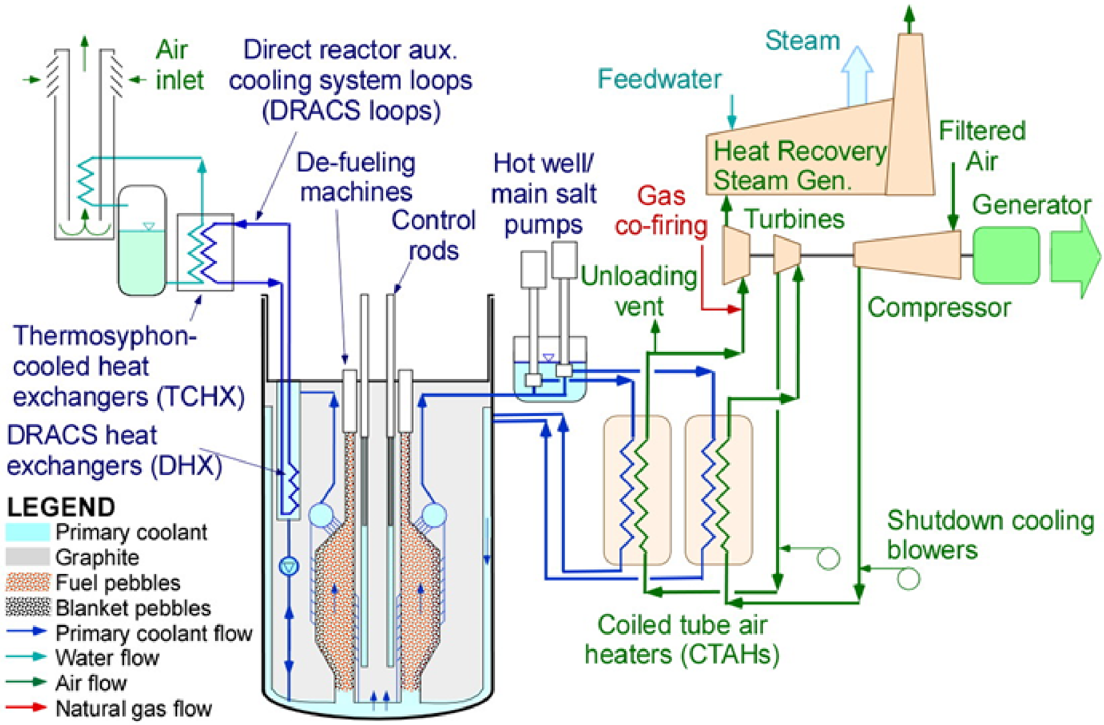

Figure 2-5 Mark 1 PB-FHR Flow Schematic [2-14]

Table 2-2 Design Parameters for FHRs

Parameter	Mk 1 PB-FHR [2-14]	AHTR [2-16]
Coolant	FLiBe	FLiBe
Power, MWt	236	3400
U enrichment, wt. %	19.9	9.0
Fuel discharge burnup, MWt-d/kg	180	71
Core power density, MWt/m^3	22.7	12.9
Fuel average surface heat flux, MWt/m^2	0.189	0.285
Passive decay heat cooling	DRACS	DRACS

The control system for the PB-FHR includes a buoyant control rod in the central reflector in a channel with salt at the inlet temperature. Any transient that increases the temperature in the channel above 615°C neutral buoyancy value causes the rod to insert. There are also shutdown blades that enter in the pebble bed. Fuel, moderator, and coolant temperature reactivity feedbacks are all negative—to the extent that anticipated transients without scram are not expected to result in any deleterious effects.

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3 SIMULATION SCENARIOS

3.1 Introduction

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 generic "licensing-basis events."

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 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 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.

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 met. For solid-fuel reactors these limits may be thermal or mechanical parameters and usually relate to the potential for fuel damage to preclude the release of fission products to the coolant. In FHR designs, since it is difficult to hypothesize temperature increases that lead to significant fission product release, there are additional acceptance criteria that relate to thermal or mechanical limits outside the fuel, for example, the temperature of the reactor vessel. For liquid fuel reactors acceptance criteria might also include 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 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 chapter 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.

However, before considering events that might need to be simulated using neutronic and thermal-fluid models, it is useful to consider a methodology for process hazard analysis. What-If analysis is one of several methods used by the Department of Energy and is said to be particularly useful for applications where experience and data are limited. This method and its application to the LFTR is described in [3-1]. Table 3-1 shows a portion of that analysis that is applicable to this pre-PIRT. Although carried out for a particular design with unique features, the results are generally applicable to each of the MSR designs.

Each question is answered in [3-1], however, the specifics of the answers are only of interest herein to the extent they provide general system behavior that would have to be simulated and can inform the discussion of events for the different molten salt reactor designs discussed in the remainder of this chapter.

Table 3-1 What if Questions Based on the LFTR [3-1]

LFTR System	What If Question
Reactor Vessel/ Containment Cell	What if unintentional control rod withdrawal occurs?
	What if loss of blanket salt occurs?
	What if premature criticality occurs during filling?
	What if the exit temperature of fuel salt from the reactor is much higher than anticipated?
	What if the inflow temperature of fuel salt is relatively cooler than anticipated? / What if inflow of fuel salt contains a “cold slug” or partially frozen salt?
	What if inflow of contaminants or unexpected isotopic ratio in the fuel salt enters the reactor core?
	What if reactor containment cell pressure is greater than designed operational range?
	What if reactor vessel pressure is greater than designed operational range?
	What if breakage of one or more graphite tubes occurs?
	What if accidental loss of fuel/coolant salt occurs?
	What if electrical resistance heaters fail to operate within reactor containment cell?
Fuel Salt Processing	What if interruptions in fuel salt flow occur?
	What if decay heat removal rates are lower than expected design rates?
	What if excess pressure accumulates in the helium bubbler (sparger) used to remove fission products from the fuel salt?
Primary Heat Exchanger	What if high pressures cause a minor failure within the primary heat exchanger?
	What if a major failure within the primary heat exchanger occurs?
	What if primary fuel pump stops operating?
	What if the sealed housing for the electric drive motors for pumps fail?

LFTR System	What If Question
Blanket Salt Processing	What if inadequate removal of Pa or U in the blanket salt occurs due to a failure of the first and/or second reductive extractive column?
	What if the electrolytic cell is improperly operated?*
	What if blanket salt chemical processing does not occur at designed flow rate?
Drain Tank	What if inadvertent thawing of the freeze valve holding fuel salt in the primary coolant loop occurs?
	What if a piece of graphite enters the drain tank when the emergency drain tank is used?
	What if improper or inadequate cooling of the drained fuel salt occurs in the event of an emergency shutdown?
	What if a partially thawed piece of the salt plug (or any other solid mass) obstructs piping to the drain tank during times of emergency shutdown?
*Examples of features that may be unique to the LFTR	

3.2 Liquid-Fuel Molten Salt Reactors

3.2.1 Normal Operation

As stated above, calculations under normal operation are necessary to show how the reactor will start up and shut down and how the control elements and additions and subtractions to the molten salt composition will affect the system. Normal operation also sets the initial conditions for most licensing-basis events and is the basis for determining the fluence on structures.

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 fissile material and possibly fertile material. 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 in some situations, as a function of location within the reactor system and containment structure (see also the discussion in Section 5.2). The degree to which this tracking is necessary will depend on the particular design.

3.2.2 Reactivity Changes

Two causes of an unwanted slow increase in reactivity could be the result of the addition of too much fissile material or the inadvertent withdrawal of control elements. These events would cause the power, and simultaneously the temperature of the fluid, to increase. It is assumed that a critical configuration can only exist in the core (as opposed to the piping where fissile material enters the system in some designs). Whether the event is due to the addition of fissile material or the withdrawal of control rods, there is a change in the spatial power distribution as the overall power increases. 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 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 slows down the exit rate of fission products, 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 the blanket. One that is unique for reactors with moving moderator rods, is the uncontrolled movement of those rods. These events would result in consequences as described above.   The loss of salt in the blanket could also be compensated for with a design (see Chapter 2) having a floating control rod in the blanket salt that would add negative reactivity as it moved further into the core as the blanket salt level dropped.

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 left unchecked, 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 are fundamentally different from solid-fuel reactors, a variety of new accident scenarios will have to be considered as part of the regulatory review. For example, a scenario [3-1] 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.

3.2.3 Increase/Decrease of Temperature

The 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.

3.2.4 Other Scenarios

Malfunctions of the decay heat removal system will need to be simulated. This includes systems that might be in the primary system or in the drain tank. However, at this point in time, insufficient information on those systems precludes their consideration. Another system whose operation may need to be simulated is the direct reactor auxiliary cooling system (DRACS) proposed for use in FHRs [3-2] and also being considered for liquid-fuel reactors [3-1].

3.3 <u>Solid-Fuel Molten Salt Reactors</u>

3.3.1 Generic Information

Solid-fuel molten salt reactors would have generic licensing-basis events in line with those that need to be considered for other solid-fuel reactors such as light water or gas cooled reactors. Hence, reactivity insertion events, power-cooling mismatches, and loss-of-coolant events all need to be analyzed. Many of the events considered for the AHTR design [3-3] shown in Figure 3-1 may be applicable to the PB-FHR as well. Hence, they are discussed herein.

For the AHTR, potential events for safety consideration (primarily from reference [3-4]) are listed below and several are discussed in more detail below. Historically, accidents have been categorized according to their approximate likelihood of occurrence into three categories: anticipated operational occurrences, design basis accidents and beyond design basis accidents. The regulatory acceptance criteria for each category have depended on the likelihood of the occurrence of the event. Because there is no regulatory precedent for how these accidents may be categorized for molten salt reactors, in the following discussion events are considered for which a confirmatory analysis thermal/hydraulics/neutronics modeling capability might be required, without consideration of how these events might be categorized. The discussion is restricted to internal events rather than external events. Although some external events, such as earthquakes and aircraft crash could lead to challenges affecting the reactivity or coolability of fuel, in general the impact of those events on primary system behavior are the same as those of comparable internally-initiated events.

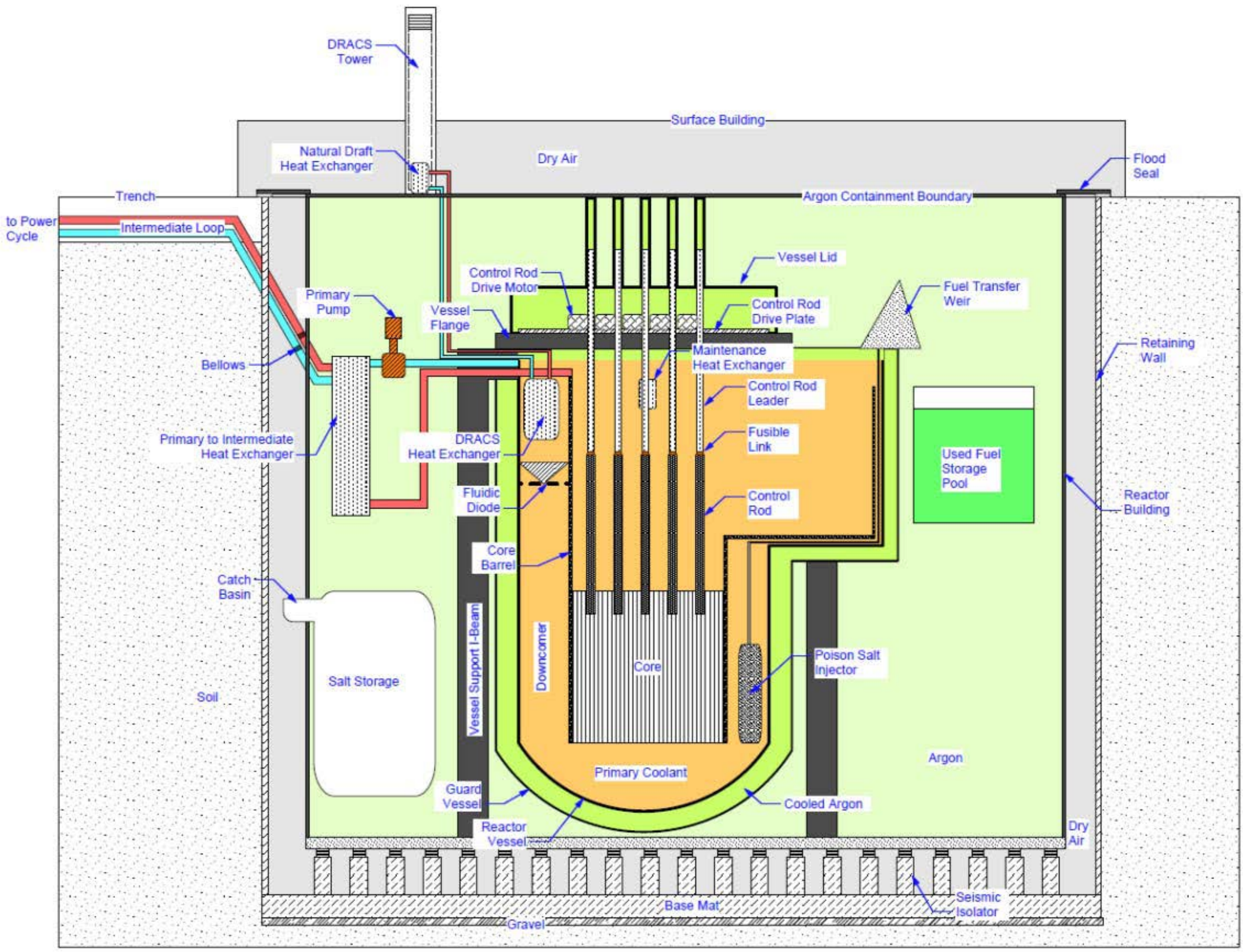

Figure 3-1 Schematic of AHTR Building Components

<u>Normal Operation</u>

- Start-up/heat-up
  - o Operator controlled increasing of reactor power to rated level. Heat-up of the primary system possibly through auxiliary heating system or through reactor power.
- Shutdown/cool-down
  - o Operator controlled decrease of reactor power down to shutdown. Possible cooling of the primary system.

- Reactivity insertion/removal (i.e., intended)
    - Operator adjustment of reactivity control such as insertion/removal of control rods.
- Power oscillations
    - Oscillations in the reactor power (e.g., possibly when bringing the core up to power)

<u>Anticipated Operational Occurrences:</u>

- Overcooling
    - Primary side (concern: time to freeze)
      From full power, the primary pumps trip, reactor trips, and the power cycle and intermediate loop pumps remain on removing heat from primary system. DRACS may or may not be assumed to operate.
    - Secondary side (concern: time to freeze)
      From full power, the primary pumps trip, reactor trips, and the secondary pumps trip but heat continues to be rejected from the intermediate loop to the ultimate heat sink.
- Heat exchanger channel rupture
    - Primary side (concern: reactivity, salt cleanup time)
      From full power, a channel in the DRACS heat exchanger or the primary-to-intermediate loop heat exchanger fails.
    - Secondary side (concern: heat removal from primary to secondary side)
      A channel fails in the heat exchanger from the intermediate loop to power conversion system. This may be evaluated at full power or shutdown conditions.
- Pump trip with coast-down (e.g., one pump) (concern: peak fuel and vessel temperatures, peak thermal stresses, core flow instabilities)
    - From full power, a single pump trips and coasts down. The reactor is assumed to trip. This may cause asymmetric flow and salt temperatures in the core region.
- Loss of load/turbine trip
    - From full power, loss of load, turbine trips and other unanticipated reactor trips will be analyzed, generally assuming auxiliary power remains available.
- Loss of primary system trace/auxiliary heating (concern: minimum salt temperature and salt freezing)
    - During shutdown, there is a loss of ability to add heat to primary system.
- Inadvertent control element movement (concern: core reactivity)
    - With the core at full power or shutdown, the control system inadvertently directs the control blades to be withdrawn improperly.

<u>Accidents</u>

- Anticipated Transient Without SCRAM (ATWS)
    - While the reactor is at full power, a transient event occurs and the primary control system fails to trip (concern: peak fuel temperature, thermal stresses, peak vessel temperatures.)
- Flow blockage (concern: peak fuel temperature, fuel thermal stresses)

- While the reactor is at full power, the entrance to an assembly is assumed to be blocked (e.g., frozen coolant, debris, impurities).
- Loss of forced cooling (LOFC) (concern: peak fuel and vessel temperature)
  - With the reactor initially at full power, all primary pumps trip, and reactor trips. Heat must be rejected through the DRACS or other available cooling systems.
- Loss-of-coolant accident (LOCA) (concern: salt level, cooling of fuel, loss of barriers to release of radioactive material, generation of combustible gases, containment integrity)
  - With the reactor starting at full power, a failure in the primary piping is assumed to occur resulting in outflow of reactor coolant with possible ingress of gas.
- Pump locked rotor (concern: margin to component failure)
  - With the reactor initially at full power, a single pump rotor is assumed to seize and stop instantly (e.g., bearing seize) and reactor trips. This may cause dynamic loadings due to pressure waves and asymmetric core conditions.
- Station blackout (concern: peak fuel temperature, peak vessel temperature, coping time, battery/other power supply duration
  - All AC power to the plant is lost including on-site diesel generators. Either demonstrate capability to reject heat passively or ability to reject heat must be reestablished prior to depletion of batteries.
- Reactor vessel breach (concern: salt level in primary system, containment integrity, environmental releases)
  - The primary vessel is assumed to fail while the reactor is at full power. One could assume the leak is detected and the reactor is scrammed or the leak remains undetected and reactor remains at power for some time. The location and size of the break should encompass a range of possible scenarios.
- Loss of ultimate heat sink (concern: coping time, peak fuel and vessel temperatures, environmental releases)
  - From full power, all DRACS systems are lost, possibly severed above ground, and heat removal via the intermediate loop is halted. Maintenance cooling loop may or may not be assumed to be available.

3.3.2 Overcooling Events

According to [3-3]: “It is possible to overcool and freeze the primary reactor coolant, the intermediate coolant, or the DRACS coolant. While used fuel remains in the reactor vessel, its decay heat makes freezing the primary coolant in the reactor vessel incredible. The primary FLiBe coolant salt has a higher melt point (458ºC) than the intermediate coolant salt KF-ZrF_4 (390ºC) [3-5]. If both the power cycle and intermediate loop pumps remain on and the primary loop pumps are turned off after reactor shutdown, the higher melt point FLiBe will freeze in the primary to intermediate heat exchangers. Similarly, if the intermediate pumps are turned off and the power cycle pumps remain on following reactor shutdown the intermediate coolant salt will freeze. While neither of these events directly damages the fuel, they both remove the normal condition heat rejection path from operation. Both automatic controls and procedures are planned to prevent inadvertent overcooling of the primary heat transport path."

"The DRACS are the last line of defense in keeping the fuel cool during an extended station blackout. As such they are a reactor safety feature and high assurance must be continuously available they are capable of performing their safety function. Under normal conditions, the DRACS will continuously reject heat and represent a small parasitic load. Instrumentation (temperature measurement) will be provided to ensure that the DRACS component temperatures remain well above freezing and that they are properly functioning." However, they can lead to overcooling as explained below for a station blackout.

3.3.3 Inadvertent Control Element Movement

According to [3-3]: "If the control system were to inadvertently direct the control blades to be withdrawn improperly, the fuel's strong negative thermal reactivity feedback would mitigate the reactivity increase. The mechanical design of the control blade drive system does not permit the control blades to be moved rapidly. In the event of a large positive temperature excursion, the passive negative reactivity insertion mechanisms (negative temperature coefficient fuel and melt point fuse controlled shutdown systems) would activate preventing fuel damage." The melt point fuse is part of each control rod mechanism in the AHTR design.

3.3.4 Primary Loop Break

According to [3-3]: "The primary loop piping connections are near the top of the reactor vessel. Both the maintenance and DRACS heat exchangers are located below the level of the primary heat exchangers, thus two independent means for removing decay heat would remain functional in the event of a primary loop detachment (double guillotine break)." Hence, it is the behavior of the DRACS that needs to be simulated.

3.3.5 Loss of Forced Flow

According to [3-3]: "If the primary coolant pumps were to fail, the reactor would first shut down either under operator control or passively. The fuel's decay heat would be removed by a combination of the maintenance cooling loop system and the DRACS. Both the maintenance cooling system and the DRACS are independently sufficient to remove the decay heat, so redundant cooling capabilities remain following the loss of primary cooling. Additionally, the maintenance cooling system's power can be manually switched to an alternate power source, so either grid or backup diesel generators could be used to provide an additional power source for cooling." This sequence is similar to what would happen if there was a loss of the ultimate heat sink.

3.3.6 Station Blackout

According to [3-3]: "In the event of a full station blackout, the reactor would first shut down either under operator control or passively. The fuel's decay heat would be removed by a combination of the maintenance cooling loop system and the DRACS. … [Each system is] independently sufficient to remove the decay heat, so redundant cooling capabilities remain following the loss of power.

"The AHTR DRACS are sized to remove 0.75% of full power under fully developed flow conditions. With a station blackout accident, the reactor temperature will initially rise and then fall again as the fuel decay heat decreases. The DRACS heat rejection rate will increase with the larger temperature difference to ambient and then decrease as the reactor cools. … Salt would begin to freeze at the cooler pipe walls in the natural draft heat exchanger and thereby decrease the heat transferred from the interior hotter salt. Significant additional modeling and experimentation will be required to demonstrate how long would be necessary for the DRACS to freeze solid given the complex interactions between the solidification, insulation, viscosity, and fluid flow rate and whether this would occur at a sufficiently long time (months) following shutdown such that the small amount of conduction and convection cooling through the vessel would keep the fuel temperature sufficiently low."

3.4 References

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4 IMPORTANT PHYSICAL PROCESSES FOR MSRs

4.1 Introduction

Phenomena are defined herein as physical processes affecting the outcome of events. In the development of simulation tools, all of the principal phenomena must be modeled. Often the form of the model is based on theory and key parameters within the model are determined experimentally. In Chapter 2, the MSR designs of interest were discussed. Since specific design details are either not known or not disclosed for most designs, in this chapter a composite design is considered with features characteristic of an amalgam of known designs. The general characteristics of scenarios that might have to be simulated were discussed in Chapter 3 but details on how these scenarios would progress are not well-known. Instead of discussing phenomena within the context of specific scenarios, the strategy selected by the panel was to first consider normal (steady state) operation. Figures-of-merit (FoMs) were defined from the viewpoint of the degree and nature of safety impact. The principal phenomena affecting steady state operating parameters were identified. For each phenomenon, the panel members made a qualitative consensus assessment of the FoMs affected by uncertainty in the ability to model that phenomenon. The panel members then considered how various transient accident scenarios would impact the overall importance of each phenomenon. Because there has recently been consideration given to the importance of phenomena in solid-fuel MSRs, the panel focused on liquid-fuel MSRs. Thus, the bulk of this chapter is devoted to understanding the importance and state of knowledge of phenomena in liquid-fuel MSR accidents.

4.2 Thermal Spectrum Liquid-Fuel MSRs

4.2.1 Neutronics Phenomena

The panel chose the figures-of-merit (FoMs) in Table 4-1 to study neutronics phenomena for thermal-spectrum liquid-fuel MSRs under normal operation. 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 includes 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 4-1 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 GDC requirement that in the power operating range the net effect of the prompt inherent nuclear feedback characteristics tends to compensate for a rapid increase in reactivity. It is noted that this FoM, 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, if they exist. Experience with the molten salt reactor experiment (MSRE) carried out at Oak Ridge National Laboratory, 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.

For each phenomenon, a definition or clarification was provided and the impact was discussed during the pre-PIRT—in particular with respect to the FoMs. The impact relates to importance without specific ranking as done in an ordinary PIRT. The path forward with each phenomenon was discussed. Finally, the significance of the phenomenon was discussed with respect to transients.

The important neutronic phenomena are listed in Table 4-2 according to two categories: basic nuclear data and material composition. Basic nuclear data means the underlying nuclear data libraries, for example ENDF/B-VII.1, that underpin a neutronic model of an MSR. Material composition means the accurate modeling of the composition of materials in the core, and throughout the primary loop, including fission and transmutation products.

Table 4-2 Neutronic Phenomena for Thermal Spectrum Liquid-Fuel MSRs

Phenomenon [Definition]	Impact	Path Forward	Comments on Transients
Basic Nuclear Data			
^{6}Li Balance [Cross sections for the production and destruction of ^{6}Li]	^{6}Li has a large absorption cross-section and is distributed uniformly but has a low impact on power distribution. Contributor to tritium in the core. FoM5.	^{6}Li absorption cross-section is well known. $^{9}Be(n,\alpha)^{6}Li$ production reaction is well known.	Not important for transients.
Moderation by fuel salt (e.g., FLiBe) [Free atom scattering cross sections for F, Li, Be, or other constituents]	FoM1. Small impact.	Inelastic scattering cross-sections for F and ^{7}Li have a high uncertainty, but low importance.	Low sensitivity.
Thermalization by fuel salt [$S(\alpha,\beta)$ for F, Li, Be, or other constituents.]	FoM1. Small impact.	Instruments do not measure this with enough precision to build a cross-section library experimentally. This could be calculated (standard practice).	Low sensitivity.
Moderation by carbon [Free atom scattering cross-sections for C]	Moderation in graphite will have major effects on k-eff and power distribution. Significant amount of C in thermal MSRs. FoM1, FoM2.	These effects are well known fundamentally.	No special consideration for transients.
Thermalization in carbon [$S(\alpha,\beta)$ in carbon/graphite]	Thermalization in graphite will have major effects on k-eff and power distribution. Significant amount of C in thermal MSRs. FoM1, FoM2.	These effects are well known fundamentally.	No special consideration for transients.

Phenomenon [Definition]	Impact	Path Forward	Comments on Transients
Moderation and thermalization by zirconium hydride [Free atom scattering cross-sections. S(α,β)]	For those reactors containing zirconium hydride there will be major effects on k-eff and power distribution. FoM1, FoM2.	These effects are well known fundamentally.	No special consideration for transients.
Absorption in fuel salt, including fission products [Absorption cross-sections for the fission products and constituents of the fuel salt (with the exception of ^{6}Li which is addressed separately)]	Wide-ranging impact over all FoMs.	These effects are generally well known; the exception being the build-up of minor actinides.	No special consideration for transients.
Absorption in carbon [Absorption cross-section for carbon]	The absorption cross-section was changed between ENDF/B7 and ENDF/B7.1 and can cause differences in excess of 1% in k-eff. There is uncertainty in the accuracy of the absorption cross-section. Some designs have large quantities of carbon. FoM1, FoM2.	Evaluation of Very High Temperature Reactor Critical (VHTRC) indicates ENDF/B7.1 resolves issues with carbon absorption cross-section.	No special consideration for transients.
Neutron production from Be [Cross-sections for (γ,n), (α,n) and (n,2n) reactions]	This may be more important for transient analysis than steady-state where delayed gammas become more important. Current codes don't account for (α,n) reactions. Large uncertainties. FoM1, FoM2, FoM4.	Calculations should be performed to resolve uncertainties in neutron production from Be.	No special consideration for transients.

Phenomenon [Definition]	Impact	Path Forward	Comments on Transients
Neutron production from F [Cross-section for (α,n) reaction]	Current codes don't account for (α,n) reactions. Large uncertainties and may be a small effect. FoM1, FoM2, FoM4.	More study is necessary to determine the impact and resolve the uncertainty.	No special consideration for transients.
Absorption in control rod materials [Absorption as a function of temperature]	Very important. FoM1, FoM2.	Measurements must be made to confirm control element worth.	No special consideration for transients.
Neutron precursor decay constants and fission yields [Generation of delayed neutrons]	Necessary for the calculation and tracking of delayed neutron precursor isotopes. FoM3.	Traditional methods may be sufficient for calculation of delayed neutron precursor behavior. Will be dependent on reactor design.	Absolutely necessary for transients, particularly long-term transients.
Fuel displacement effect [Reactivity control through the displacement of salt fuel]	Very important. FoM1, FoM2.	Very design dependent.	No special consideration for transients.
Material Composition			
Carbon density due to dimensional change [Changes in the density of C components due to swelling]	Dimensional change effectively diverts molten salt outside core. FoM1, FoM2.	Actual behavior of the material is outside the scope of the pre-PIRT.	No special consideration for transients.
Depletion of control rods [Depletion of control rod materials, including the in-core residence time and depletion chains for control materials]	Liquid fuel has low excess reactivity so rods can be operated mostly withdrawn and hence low depletion. FoM1, FoM2.	Not important to pursue unless a design keeps some rods inserted.	May affect the unprotected transient over-power and shutdown margin. Relatively low impact. Design dependent.
Spectral history effects [Depletion accounting for presence of control rods or other spectrum changing asymmetries]	Spectral history effects are the result of core average spectrum as a function of time. FoM1, FoM2.	Depletion methods are well known.	No special consideration for transients.

Phenomenon [Definition]	Impact	Path Forward	Comments on Transients
Isotopes to track [Which isotopes to track in depletion simulations]	This could be an issue from a computational overhead and memory standpoint. FoM1, FoM2, FoM3.	Would need to perform a sensitivity study to determine which isotopes to track. Design and operation of isotope control systems will affect the analysis.	No special consideration for transients.

4.2.1.1 Basic Nuclear Data Phenomena

^{6}Li Balance: The panel identified several important data sets related to ^{6}Li. 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 in thermal spectrum fluoride salt MSRs. ^{6}Li has a large absorption cross-section; it is distributed uniformly and has a low impact on power distribution. This quantity directly impacts FoM5 and the tritium source term, and 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 moderation and thermalization of neutrons by the fuel salt will directly impact FoM1. Overall, this is expected to have a relatively small impact. The scattering cross sections for F and Li have a low contribution to overall eigenvalue uncertainty and low sensitivity in thermal spectrum MSRs [4-1]. For thermalization, S(α,β) libraries for F, Li, and Be in FLiBe have been developed and are undergoing testing [4-2].

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 thermal MSR 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, this will have major effects on reactivity (FoM1) and power distribution (FoM2). These effects are reasonably well understood, and can leverage experience from TRIGA reactors.

Neutron Absorption by Carbon: The absorption cross-section was changed between ENDF/B-VII.0 and ENDF/B-VII.1, as shown in Figure 4-1. 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 [4-3]. 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.

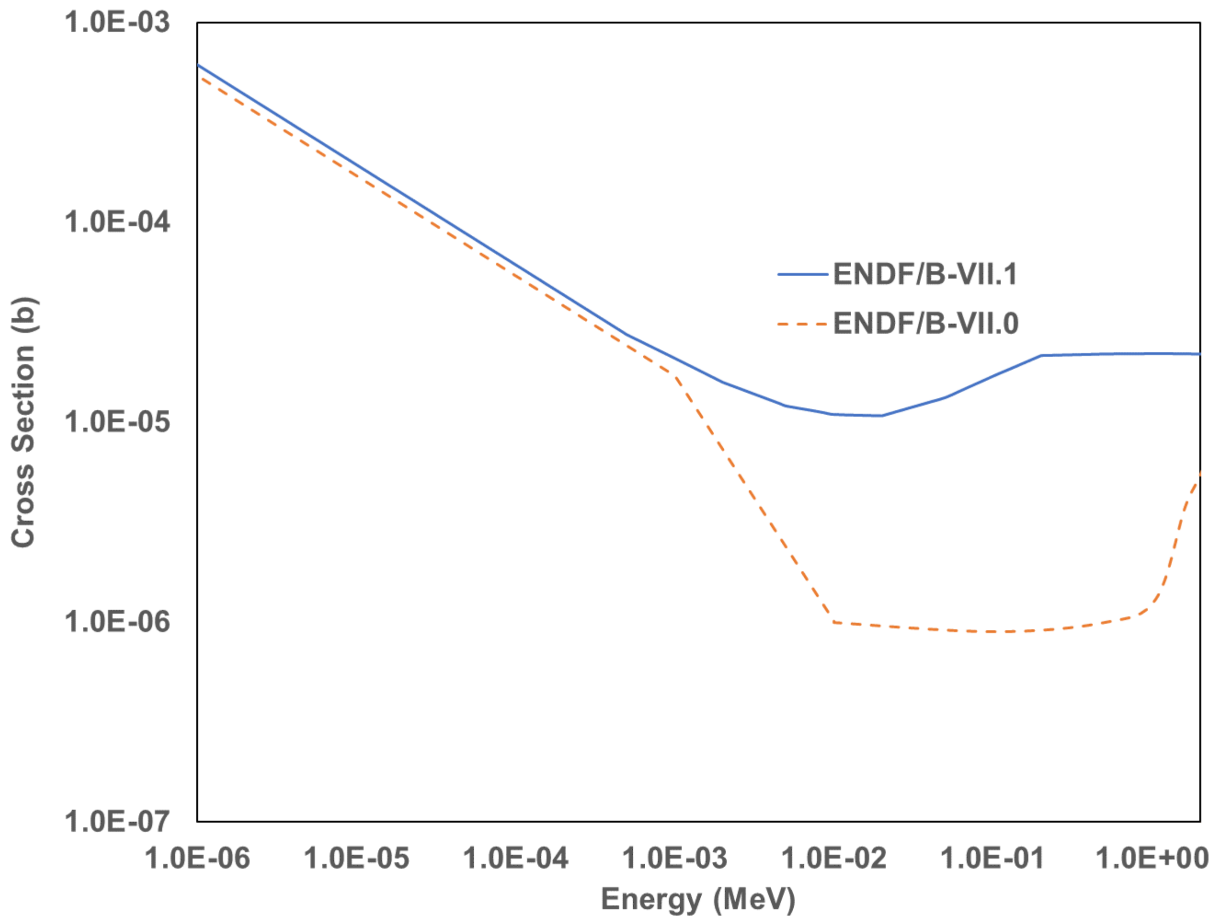

Figure 4-1 Differences in ^{12}C Neutron Absorption Cross Section Evaluations

Neutron Production from Beryllium and Fluorine: This phenomenon includes neutron production in beryllium from (γ,n), (α,n) and (n,2n) reactions. These data may be more 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 [4-4], 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 [4-5]. Recent estimates for the Chinese FHR test reactor indicate about 4 pcm of impact from beryllium photoneutrons [4-6]. 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.

Absorption in Control Rod Materials and Fuel Displacement: This is absorption in control rod materials, if present in a particular design, as 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 can be made to confirm the calculated control element worth.

Neutron Precursor Decay Constants and Fission Yields: These phenomena include production of delayed neutrons in the reactor core and throughout the primary loop. 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.

4.2.1.2 Material Composition Phenomena

Carbon Density Due to Dimensional Change: This includes changes in the density of carbonaceous components due to dimensional change, including 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. The actual 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 directly impacts FoM1-FoM4.

Depletion of Control Rods: This includes 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 within the cycle for reactivity control. For those designs that employ frequent control rod insertion, this may impact the progression of unprotected transient over-power and shutdown margin.

Operational History Effects: This is depletion accounting for 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 also closely coupled to the operational history effects. The design and operation of isotope control systems will directly impact the analysis and conclusions. This is a design dependent issue. One key outcome of this study is that a separate tool is needed to track MSR chemistry, composition, and isotopes. This includes online removal of fission products (passive or active), online feed 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.

4.2.2 Thermal-Fluid Phenomena

The figures-of-merit against which the significance of phenomena are evaluated are related to the potential for radioactive material release or the loss of a barrier to release. For liquid-fuel MSRs, the barriers to release of radioactive material are substantially different from those of the solid-fuel reactors historically licensed by the NRC. The first two barriers to release of radioactive material from a solid-fuel reactor, the matrix of the fuel and the fuel clad, do not exist for liquid-fuel reactors. For the liquid-fuel MSRs it is assurance of the integrity of the primary system boundary and containment boundary that have high importance in controlling the magnitude of radioactive material release to the environment in postulated accident scenarios.

It is assumed that the confirmatory safety analysis for a design-basis or beyond design-basis event will also require the development of tools to model the changes of fuel composition and radioactive material inventory that occur as a function of operating time. However, for the present exercise it is assumed that limiting conditions will be provided as input data to the safety analysis of an event.

In the pre-PIRT, the initial evaluations were performed for steady state operation, even though the principal concern of confirmatory analyses will be associated with dynamic licensing basis events. However, accident transient analysis begins from a steady state initial condition and the thermal-hydraulic analysis requirements at a minimum must address steady state requirements.

Relative to LWR safety analysis, for MSRs the lack of high pressure operation, energetic break flow, rapid system depressurization, core uncovery, reflood and two-phase flow simplify the thermal-hydraulic aspects of the safety analysis. However, the multi-dimensional flow distribution may be more complex in the MSR pool-type as opposed to loop-type designs. The potential plate-out of materials from the salt on heat transfer surfaces is an area of significant uncertainty. Freezing of salt in over-cooling transients can also be a concern in MSRs but for liquid fueled MSRs the presence of decay heat in the salt reduces that potential. If lithium hydride is used as a moderating material in the design, additional experimentation will be required to determine the stability of the hydride under irradiation. For thermal spectrum liquid fuel MSR designs the pre-PIRT did not identify significant issues associated with the current state of knowledge of material properties or flow parameters.

The panel chose the figures-of-merit in Table 4-3, which are applicable to both thermal spectrum and fast spectrum liquid-fuel MSRs. The objective of safety analysis is to demonstrate the capability of the inherent safety characteristics of the plant augmented by engineered safety systems to assure an adequate level of protection to the public against the consequences of accident scenarios. The level of protection required depends on the likelihood of the different possible accident scenarios. Traditionally, the consequences of accident scenarios are measured in terms of radiological exposure. This aspect of the pre-PIRT study addresses the state of knowledge associated with the phenomena considered in the thermal-hydraulic component of safety analysis. The release and transport of radioactive material depend directly on the thermal-hydraulic response of the system. Thus, in the identification of different figures-of-merit associated with the existing ability to model thermal-hydraulic phenomena, the panel considered how those phenomena could impact radiological exposure in accident scenarios.

Table 4-3 Figures-of-Merit for Liquid-Fuel MSR Thermal-Fluids

Figure-of-Merit	Definition
FoM1: Primary System Temperature Distribution (Core Inlet and Outlet Temperature)	Salt temperature distribution throughout the core and flow loops. Fluid temperature at the inlet and outlet of the core are of particular interest.
FoM2: Power Distribution and Peak Power	Total power and power distribution generated from fission in the salt.
FoM3: :Flow Velocity	Salt flow velocity, primarily bulk flow velocity but potentially also local velocities.
FoM4: :Liquid Composition and Distribution	Salt chemical and isotopic composition throughout the core and flow systems. This could be time dependent.
FoM5: Gas Transport and Composition	Includes the transport of tritium, fission gases, and any gases generated or those added for operational purposes to the core for moderation or chemistry control.
FoM6: Solid Phase Composition and Distribution	The processes of species solubility, plate-out, fouling, solid particulate formation and transport.

FoM1 addresses the primary system temperature distribution. At the simplest level the core inlet and core outlet temperatures represent the minimum and maximum temperatures within the primary system. The safety-related concerns are associated with: 1) temperatures leading to fission product evolution from the salt, 2) temperatures leading to fission product and corrosion plate-out on surfaces, and 3) temperatures of structures leading to the potential for creep or failure. Salt temperature also affects feedback to neutronics calculations.

FoM2 relates to power distribution including peak power. This includes neutron and gamma heating in moderator, reflector and structural components. The total power and power distribution generated from fission in the salt as a function of time in the scenario affect the potential for radioactive material release and transport, heat removal to the ultimate heat sink, and the potential for freezing of salt.

FoM3 is associated with flow velocity. It affects the processes of species solubility, plate-out, fouling, solid particulate formation and transport. Flow distributions in the core could result in locally higher power production, erosion of components, or gas (e.g., tritium) transport. Other safety concerns are associated with the precipitation of species that could negatively impact operating safety margins.

FoM 4 is associated with salt chemical and isotopic composition throughout the core and flow systems. This could be time-in-cycle dependent. Safety concerns are associated with effects on 1) reactivity, 2) power distribution and 3) redox potential.

FoM 5 addresses gas transport and composition. It includes the transport of tritium, fission gases, and any gases generated or added to the core for moderation or chemistry control. The consequences of postulated accident scenarios are directly associated with the release and transport of radioactive or hazardous material.

FoM 6 is associated with solid-phase processes. Safety concerns are associated with uncertainties regarding multi-component phase diagrams and the precipitation of species that could negatively impact operating safety margins.

Table 4-4 provides the assessment by the panel members of the state of knowledge of thermal-fluid phenomena for thermal spectrum, liquid-fueled MSRs. The assessment was performed within the context of the ability to model steady state conditions and then, as an ancillary activity, for the analysis of transient scenarios. The phenomena are specified for five categories: fuel salt, core materials, vessel/piping, primary pumps, and primary heat exchanger. They are then discussed according to whether they are physical properties, or heat transfer or fluid flow phenomena.

Table 4-4 Thermal-Fluid Phenomena for Thermal Spectrum Liquid-Fuel MSRs

Phenomenon [Definition]	Impact	Path Forward	Comments on Transients
Fuel Salt			
Physical properties - Heat capacity of fuel salt (e.g., FLiBe) [As a function of temperature, composition]	Fundamental to simulation of steady temperature and flow distribution. Directly impacts axial temperature profile in salt as it flows through core region and the steady state temperature of structures. FoM1	The properties of FLiBe and other salts must be measured over the range of expected conditions.[c] Heat capacities of fluoride salts are well known (within a few percent).	Range of conditions for which properties must be known is expanded but for fluoride salts uncertainty is small. Has a potentially larger impact on power/cooling mismatch events than on steady state.
Physical properties - Thermal conductivity of fuel salt. [As a function of temperature, composition]	Fundamental to molten salt simulation of thermal-hydraulic conditions, e.g. FoM1, FoM2	Thermal conductivity has a greater uncertainty than heat capacity. Fluoride fuel salt thermal conductivities are known to within 10-15%. LiF-NaF-KF needs further investigation. Karlsruhe Institute of Technology has conducted extensive thermo-physical property measurement for fuel salts.	Range of conditions for which properties must be known is expanded beyond that for the steady state.

[c] In [4-7] R. Romatoski presents results of a review in her doctoral research of the uncertainties in the physical properties of key fluoride salts.
LiF-BeF: density – 2%; heat capacity – 3%; thermal conductivity – 10%; viscosity – 20%
NaF-ZrF_4: density – 5%; heat capacity – 20%; thermal conductivity – 15%; viscosity – 20%
LiF-NaF-KF: density – 2%; heat capacity – 10%;

Phenomenon [Definition]	Impact	Path Forward	Comments on Transients
Physical properties - Viscosity of fuel salt. [As a function of temperature and composition]	FoM1, FoM2, FoM3	The properties of FLiBe and other salts must be measured over the range of expected conditions. Values of FLiBe properties vary by ~20% in preferred correlation.	Range of conditions for which properties must be known is expanded. Increased importance in natural circulation and for timing of transition to natural circulation.
Physical properties - Coefficient of thermal expansion of fuel salt. [As a function of temperature, composition]	Determines flow characteristics, particularly in natural convection, neutronic behavior and reactivity feedback coefficients, FoM1, FoM2, FoM3, FoM4	Can calculate density with quasi-chemical models to less than 10%.	Important to over-power transients due to reactivity feedback and transients that require passive decay-heat removal, as a driver of natural circulation
Heat transfer coefficient to core structure. [Under forced/natural convection. Need to consider moderators and other core structures]	Under steady state, not very important. Becomes more important under accident conditions. FoM1.	Single phase heat transfer is well understood and can be calculated to within 10%. Forced convection is better understood than natural circulation heat transfer.	May be important due to impact on controlling heat release from internal structures back to the fuel salt and controlling heat transfer during an event. Affects margin to limiting temperature conditions for core structures.
Heat transfer coefficient to piping/vessel in primary circuit [Under forced/natural convection. Does not include heat exchanger]	Has an impact on tritium release through the wall and corrosion. FoM5, FoM6.	Single phase heat transfer is well understood and can be calculated to within 10%. Forced convection is better understood than natural circulation heat transfer.	May be important due to impact on controlling heat release back to the fuel salt and controlling heat transfer during an event. Affects approach to limiting conditions for core structures.
Heat transfer to heat exchanger [Under forced/natural convection. Dependent on plated-out materials]	Impacts all FoMs.	Well understood absent fouling. Heat exchanger design will have an impact on heat transfer performance and prediction capability.	See "Primary Heat Exchanger" system below.

Phenomenon [Definition]	Impact	Path Forward	Comments on Transients
Fouling / Plate-out [Precipitation and collection of contaminants on heat exchanger surfaces. Corrosion, fission products, and fissile material are the sources of fouling. Time, location, and operation dependent.]	Increases the resistance to heat transfer, fluid flow. FoM1	Need to develop a predictive method to determine the rate of deposition, deposition composition, and impact on heat transfer coefficient.	May be important to over-cooling events in which fissile materials will plate-out at coldest locations (e.g. heat exchanger).
Form loss coefficients [Loss coefficients as a function of area ratio and Reynolds number]	Fundamental to molten salt simulation. Determines the flow rate. FoM3.	Can only be modeled when design is known. Form loss coefficients are generally well understood.	Potentially important to low and natural circulation flows.
Wall friction [Dependent on surface conditions, Reynolds Number]	Fundamental to molten salt simulation. Determines the flow. FoM3.	Need to know surface condition (roughness, plated-out material) as well as the shape of the passages.	Potentially important to low and natural circulation flows. Requires characterization over a larger range of Reynolds numbers.
Salt freezing [Temperature at which the salt solidifies. Dependent on composition]	Impact on steady state will be low unless part of the reactor design. Larger impact on transients. FoM6.	The melting point is relatively easy to measure, but it may be dependent on composition.	May become important for over-cooling events.
Particulate formation [Result of conglomeration of quasi-noble fission products]	Causes surface degradation due to abrasion. FoM3, FoM6.	Reduce by design or mitigation practices. Path forward depends on design details.	May become important for over-cooling events.
Entrainment of cover gas [Noncondensible gas bubbles ingested into fuel salt]	Design specific: FoM2, FoM5,	Design dependent. Can be evaluated by experiment.	May become important to pump overspeed events.

Phenomenon [Definition]	Impact	Path Forward	Comments on Transients
Multi-dimensional flow. [Need for three-dimensional flow modelling within pool.]	Design detail dependent. Computational fluid dynamics may be required to accommodate asymmetric conditions within plena. Affects all FoMs.	Design dependent.	Design dependent. Transient could increase asymmetry of flow.
Fuel salt volatility [Transport of fission products and fissile material through evaporative processes]	FoM1, FoM2, FoM4, FoM5	Requires experiments to determine volatility of fuel salts. Some data are available.	Transients will drive more volatile material into the gas space.
Core Materials			
Physical properties - Thermal conductivity of core materials [Conductivity as a function of temperature and irradiation. Includes mechanical support elements, moderator components, control elements]	Contributor to steady-state behavior. FoM2 (moderator only)	Material properties are generally well known.	May impact heat release during transients. Range of conditions for which properties must be known is expanded and time history may become important.
Physical properties - Heat capacity of core materials [Heat capacity as a function of temperature. Includes mechanical support elements, moderator components, control elements]	Low impact in steady-state. FoM6	Material properties are generally well known.	May impact stored energy during transients. Range of conditions for which properties must be known is expanded and time history may become important.

Phenomenon [Definition]	Impact	Path Forward	Comments on Transients
Thermal expansion coefficients of core materials [Thermal expansion coefficient as a function of temperature and irradiation. Includes mechanical support elements, moderator components, control elements]	Affects geometry and stresses in structural materials. FoM6	Material properties are generally well known.	Not necessarily more important for transients.
Geometry [Physical dimensions and configuration of the core materials. Includes swelling and deformation]	Surface area and flow area changes are important for all FoMs.	Geometry is dependent on design. Geometric changes must be taken into account.	Will need assurance that transients do not cause adverse changes in geometry. Control rod movement may cause flow geometry change.
Relevant properties of ZrH [Hydrogen retention as a function of temperature, swelling]	Impact is on the chemistry of the fuel salt, clad failure. In steady-state, the important FoM is FoM2.	Design the reactor to avoid cladding failure.	Will need assurance that transients do not cause adverse changes to ZrH properties.
Direct energy deposition [Fraction of energy assumed to be deposited at site of core structures]	FoM2.	Gamma energy is known fraction but location of deposition not known, but can be modeled.	May be important in over-power transients.
Tritium generation, transport, uptake, and release [Tritium contained in the structural materials]	Important phenomena in steady-state operation. FoM4, FoM5.	Develop/implement tritium transport models.	Tritium release becomes significant at high temperatures.
Vessel/Piping			
Metal and liner physical properties [Density, specific heat, and thermal conductivity of piping and vessel material]	Affects stored energy of surrounding structures. Impacts FoM5.	Metal and graphite properties are generally well known. Other material properties must be provided.	May impact stored energy during transients. Range of conditions for which properties must be known is expanded and time history may become important.

Phenomenon [Definition]	Impact	Path Forward	Comments on Transients
Piping/vessel failure modes [Includes aging effects, corrosion, thermal and mechanical stresses, radiation damage]	Inadequate assurance of structural integrity could lead to requirement for a guard vessel. FoM6.	Potential for developing failure models based on material behavior.	May initiate failure.
Insulation properties [Resistance to heat transfer to containment environment]	Affects heat loss. FoM1	Material properties are generally well known. Design information on the insulation must be provided.	Potential influence on fuel salt solidification. Could represent an initiating event. Insulation properties are important to natural circulation.
Mixing in upper plenum [Thermal striping causing three-dimensional temperature distributions on the structure. Potentially time-varying.]	Input necessary for material analysis. Impacts structures in the upper plenum and downstream. Also FoM1.	Detailed evaluation or nodalization studies may be necessary to resolve temperature distribution.	Potentially important to transients. Must be able to calculate temperature distribution in the upper plenum.
Mixing in lower plenum [Flow distribution into the individual channels.]	Non-uniform graphite aging. FoM1, FoM2, FoM3.	Detailed evaluation or nodalization to resolve temperature distribution.	Calculation of the temperature in the vicinity of the freeze plug may be important.
Direct energy deposition [Fraction of energy assumed to be deposited in vessel and piping materials]	Need to know where energy is deposited. FoM1, FoM2. Also possible effect on maintenance operations. Impacts FoM5.	Gamma energy is known fraction but location of deposition not known, but can be modeled.	Similar importance to steady-state. Contribution from plated-out fission products may become significant.
Primary Pumps			
Pump performance [Relationship between driving force, flow rate, and efficiency as a function of temperature and salt composition]	Pump working condition is included in the initial conditions in modeling for all events. FoM3.	Vendor supplied information	Will require coastdown characteristics.

Phenomenon [Definition]	Impact	Path Forward	Comments on Transients
Pump resistance or K factor [Pressure drop across pump]	Pump is an additional flow resistance when not working. Low impact on steady-state operation. FoM3.	Vendor supplied information	Will need to determine a locked-rotor k factor and variation as a function of Re.
Gas entrainment in pump [Sweep-out of gas space by the pump into the fuel salt]	Impacts reactivity if gas is forced into the core. FoM1-FoM5.	Develop gas entrainment models and bounding analysis for normal operation based on vendor-supplied information.	Not an issue for pump trip. May be important in pump overspeed transient.
Pump cavitation [Gas evolution in pump leading to vibrations.]	Impacts reactivity if gas is forced into the core. Degrades pump performance and lifetime. FoM1-FoM5.	Develop appropriate flow models for cavitation.	Not an issue for pump trip. May be important in pump overspeed transient.
Primary Heat Exchanger			
Primary side convective heat transfer. [Under forced/natural convection. Dependent on plated-out materials.]	Impacts all FoMs.	Heat transfer to the heat exchanger absent fouling is well understood. Heat exchanger design will have an impact on heat transfer performance and prediction capability.	May be important in natural circulation. Highly dependent on event and design.
Secondary side convective heat transfer [Under forced/natural convection]	Impacts all FoMs.	Heat transfer to the heat exchanger absent fouling is well understood. Exotic secondary-side fluid properties, if any, will need to be determined. Heat exchanger design will have an impact on heat transfer performance and prediction capability.	Highly dependent on event and design.

Phenomenon [Definition]	Impact	Path Forward	Comments on Transients
Primary side flow resistance [Combined wall and frictional drag across the primary side of the heat exchanger.]	FoM1, FoM3.	Vendor-supplied information.	May be important in natural circulation. Highly dependent on event and design.
Conduction through heat exchanger surfaces [Net resistance of heat exchange surface, including fouling layers. Conduction through the wall materials.]	FoM1, FoM3.	Model, assuming surface and metal properties.	May be important in natural circulation. Highly dependent on event and design.
Fouling and plate-out [Precipitation and contaminants collecting on heat exchanger surfaces. Corrosion, fission products, and fissile material are the sources of fouling. Time, location, and operation dependent.]	Increases the resistance to heat transfer, fluid flow. FoM1, FoM3.	Need to develop a predictive method to determine the rate of deposition, deposition composition, and impact on heat transfer coefficient.	Highly dependent on event and design. Could be treated as additional heat transfer resistance during transients. Additional plate-out during an over-cooling transient has the potential for actinide deposition.
Tritium diffusion through heat exchanger surfaces [Transport of tritium from primary to secondary side.]	FoM4, FoM5.	Develop tritium diffusion model. Consider plated-out layers.	Could increase/decrease in transients. Potential release of stored system tritium.

4.2.2.1 <u>Physical Properties Phenomena</u>

Thermophysical properties are necessary to evaluate energy and momentum transport in the salt and these properties must be known over the range of temperatures the salt will experience in normal operation, accident scenarios, and shutdown. Because the salts can be mixtures of more than one salt compound and the salt composition can change as fission product and possibly corrosion products are generated, parameters affected by the salt composition must also be known. In general, there are two categories of physical properties of interest for a salt: thermal-hydraulic and thermodynamic phase equilibrium. Thermal-hydraulic properties are important for transport phenomena, while phase equilibrium is necessary for thermodynamic equation-of-state and solubility.

Thermal-Hydraulic Properties: The physical properties of primary interest identified by the panel members are heat capacity, thermal conductivity, viscosity, and optical transparency. Surface tension is another property of potential importance for bubble transport. Thermal conductivity and viscosity can be strong functions of temperature. In general, the physical properties of the fluoride salts are known with reasonable accuracy, while chloride salt properties are not well known. The physical properties of common structural materials such as steels are also well known.

Phase Diagrams: Because the fluids that are used in MSR designs are mixtures of salts, it is essential to know the equations of state of not only the components but also the phase diagrams of the mixtures, particularly as they begin to solidify and constituent solids begin to come out of solution. Information necessary includes melting and boiling points as a function of salt composition, density, solubility, and liquid-vapor equilibrium.

4.2.2.2 <u>Heat Transfer Phenomena</u>

Conductive Heat Transfer within Structures: Transient conductive heat transfer within structures is a well-known phenomenon that treats heat transfer as a diffusion process based on the physical properties of thermal conductivity and heat capacity.

Heat Transfer between Fluid and Structures: Based on the properties of the fluid and structure, the contributions of convective heat transfer, conduction, and radiation can be determined from existing correlations based on the physical properties and flow rate of the fluid. These correlations are typically based on dimensionless groups such as the Reynolds, Raleigh, and Prandtl numbers.

4.2.2.3 <u>Flow Phenomena</u>

Transient flow is analyzed in reactor accidents using methods that approximate fluid behavior satisfying conservation laws (mass, energy and momentum) and other constitutive relationships for multi-component flow. Typically, it is necessary to couple the flow analysis with both the thermal behavior and neutronic behavior of the system.

The complexity of the flow analysis depends on the dimensionality of the flow and the flow regimes encountered.

Forced Flow: This refers to flow within a circuit that depends on a balance between a driving force (head) associated with a motive force (pump) and pressure losses such as those associated with friction, dissipative losses and accelerations and deceleration associated with changes in flow geometry. Solution techniques can depend on the dimensionality of the flow and the flow regime.

Natural Circulation: This refers to flow within a circuit that depends on density differences within the circuit. For events in which pump-driven flow is lost, the transition to natural circulation can lead to high fluid temperatures, particularly if the flow changes direction between pumped flow and natural circulation flow.

Form Losses: This refers to the resistance to flow resulting from changes in geometry (expansion, contraction, turns) that lead to increased turbulence and the conversion of mechanical energy to heat. Loss coefficients for characteristic changes in geometry are available in the literature. However, for complex geometries, such as the core structure in a solid-fueled reactor, loss coefficients are obtained in simulation experiments using the actual geometry.

Frictional Losses: This refers to the resistance to flow associated with the frictional interaction between the fluid and its interaction with the structure. Frictional losses are well studied for different flow regimes. Coefficients are tabulated as a function of Reynold’s number and surface roughness. Deposition on surfaces prior to or during the course of an accident changes the magnitude of the frictional loss coefficient.

Flow Regimes: Flow in pipes is characterized as laminar, turbulent or transitional, which affect pressure loss. Depending on the plant design features and accident scenario, it may be necessary to consider two-component flow such as gas bubbles within a fluid salt or flocculent solids coming out of solution. Other characteristics of the flow that may have to be modeled include turbulent kinetic energy, turbulent dissipation and the specific interfacial surface area of bubbles.

4.3 <u>Fast Spectrum Liquid-Fuel MSRs</u>

4.3.1 Neutronics Phenomena

The panel chose the figures-of-merit in Table 4-5 for neutronics phenomena for a fast spectrum MSR. The list of FoMs is very similar to the FoMs for the thermal spectrum MSRs (see Section 4.2.1) with the primary difference in 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.

Table 4-5 Figures-of-Merit for Fast Spectrum MSR Neutronics

Figure-of-Merit	Definition
FoM1: Reactivity	Net reactivity and control element reactivity.
FoM2: Power Distribution / Peak Power	Total power and power distribution generated from fission in the salt. This includes neutron and gamma heating in the reflector/shield 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	This includes the transport of fission gases, and any gases generated or added to the core for reactivity or chemistry control. Tritium considered a minor contributor.

The important neutronic phenomena are listed in Table 4-6. As with the thermal spectrum reactors, basic nuclear data and material composition are two of the important categories of phenomena.

Table 4-6 Neutronic Phenomena for Fast Spectrum Liquid-Fuel MSRs

Phenomenon [Definition]	Impact	Path Forward	Comments on Transients
Basic Nuclear Data			
Cross sections for sulfur production [Chlorine transmutation]	Corrosive nature of sulfur. No direct impact on FoMs.	Tracking of chlorine isotopic inventories	May be an initiator, but otherwise no special consideration.
Scattering by fuel salt [Free atom scattering cross sections for fuel salt]	FoM1. Small impact.	Scattering cross-sections for salt fuels are well understood. Low sensitivity.	Low sensitivity.
Absorption in fuel salt, including fission products [Absorption cross-sections for the fission products and constituents of the fuel salt. ^{35}Cl is particularly important]	Impact on all FoMs. Fission products have much less of an impact on a fast spectrum.	These effects are generally well known.	No special consideration for transients.
Absorption in actinides [Absorption cross-section for actinides, either generated in or added to the fuel salt]	Impacts breeding ratio and reactivity coefficients. FoM1, FoM3.	Cross sections for minor actinides have a high uncertainty, but the impact may be low.	Delayed neutron fraction, which is already small, is further reduced by transuranic actinide presence.
Absorption in control rod materials [Absorption as a function of temperature]	No impact--no control rods present--only shutdown rods.	Measurements will be made to confirm element worth of shutdown rods.	No special consideration for transients.
Neutron precursor decay constants and fission yields [Generation of delayed neutrons]	Necessary for the calculation and tracking of delayed neutron precursor isotopes. FoM3.	Traditional methods may be sufficient for calculation of delayed neutron precursor behavior. Will be dependent on reactor design.	Absolutely necessary for transients, particularly long-term transients.
Fuel movement [Reactivity control through the displacement of salt fuel]	Very important. FoM1, FoM2.	Design dependent.	No special consideration for transients.

Phenomenon [Definition]	Impact	Path Forward	Comments on Transients
Reflector and shield cross sections [Absorption/scattering cross sections for the reflector and shield elements]	Important because leakage is how reactivity may be controlled. FoM1, FoM2.	Dependent on materials comprising the reflector and shield. Cross sections are generally well known.	No special consideration for transients.
Material composition			
Reflector/shield material density [Changes in the density of the reflector/shield components due to thermal expansion]	Dimensional change effectively diverts molten salt outside core and alters the leakage. FoM1	Material properties are generally well known. Material properties must be provided by the applicant or determined experimentally.	No special consideration for transients.
Fuel salt density [Overall fuel salt density, including any gas bubbles present. Function of temperature and gas presence]	Important for proving fast negative feedback. FoM1, FoM2, FoM3.	Feedback mechanisms and the effects of gas bubbles on reactivity must be determined.	Feedback effects are more important in transient analysis.
Operational history effects [Fuel salt composition, accounting for operational history]	Operational history effects are the result of core average spectrum as a function of time. Determines composition of fuel salt. FoM1, FoM2, FoM3.	May be necessary to develop a method to determine operational history and salt composition at the start of a transient. Would need to perform a sensitivity study to determine which isotopes to track. Design and operation of isotope control systems will affect the analysis.	No special consideration for transients.

4.3.1.1 Basic Nuclear Data Phenomena

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 may 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 transuranic actinide presence.

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 Core Reflector and Shield Cross Sections: These are absorption and scattering cross sections for the reflector and shield elements. These cross sections 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 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.

4.3.1.2 Material Composition Phenomena

Reactor Core 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. Unknown material properties must be provided by the applicant or determined experimentally with appropriate qualification.

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: No special or unique considerations for fast MSRs relative to thermal MSRs.

4.3.2 Thermal-Fluid Phenomena

The FoMs for fast spectrum thermal fluid phenomena as defined in Table 4-7 are the same as those for thermal spectrum thermal-fluid phenomena.

Table 4-7 Figures-of-Merit for Fast Spectrum MSR Thermal-Fluids

Figure-of-Merit	Definition
FoM1: Primary System Temperature Distribution (Core Inlet and Outlet Temperature)	Salt temperature distribution throughout the core and flow loops. Fluid temperature at the inlet and outlet of the core are of particular interest.
FoM2: Power Distribution and Peak Power	Total power and power distribution generated from fission in the salt.
FoM3: Flow Velocity	Salt flow velocity, primarily bulk flow velocity but potentially also local velocities.
FoM4: Liquid Composition and Distribution	Salt chemical and isotopic composition throughout the core and flow systems. This could be time dependent.
FoM5: Gas Transport and Composition	Includes the transport of tritium, fission gases, and any gases generated or those added for operational purposes.
FoM6: Solid Phase Composition and Distribution	The processes of species solubility, plate-out, fouling, solid particulate formation and transport.

FoM1 addresses the primary system temperature distribution. At the simplest level the core inlet and core outlet temperatures represent the minimum and maximum temperatures within the primary system. The safety-related concerns are associated with: 1) temperatures leading to fission product evolution from the salt, 2) temperatures leading to fission product and corrosion plate-out on surfaces, and 3) temperatures of structures leading to the potential for creep or failure. Salt temperature also affects feedback to neutronics calculations.

FoM2 relates to power distribution including peak power. This includes neutron and gamma heating in moderator, reflector and structural components. The total power and power distribution generated from fission in the salt as a function of time in the scenario affect the potential for radioactive material release and transport, heat removal to the ultimate heat sink, and the potential for freezing of salt.

FoM3 is associated with flow velocity. It affects the processes of species solubility, plate-out, fouling, solid particulate formation and transport. Flow distributions in the core could result in locally higher power production, erosion of components, or gas (e.g., tritium) transport. Other safety concerns are associated with the precipitation of species that could negatively impact operating safety margins.

FoM 4 is associated with salt chemical and isotopic composition throughout the core and flow systems. This could be time-in-cycle dependent. Safety concerns are associated with effects on 1) reactivity, 2) power distribution and 3) redox potential.

FoM 5 addresses gas transport and composition. It includes the transport of tritium, fission gases, and any gases generated or added to the core for moderation or chemistry control. The consequences of postulated accident scenarios are directly associated with the release and transport of radioactive or hazardous material.

FoM 6 is associated with solid-phase constituents and their associated processes. Safety concerns are associated with uncertainties regarding multi-component phase diagrams and the precipitation of species that could negatively affect operating safety margins.

The thermal-fluid phenomena of interest are given in Table 4-8 and are similar to those for thermal spectrum MSRs and hence, the explanation of the phenomena in Section 4.2.2 is relevant. The relative importance to safety analysis of the different phenomena and the state of knowledge of phenomena are different, however. In general, the phenomena that must be modeled in performing the confirmatory assessment of fast spectrum reactors are less well-known than for thermal-spectrum reactors because these designs have received less attention by design organizations in the past.

Table 4-8 Thermal-Fluid Phenomena for Fast Spectrum Liquid-Fuel MSRs

Phenomenon [Definition]	Impact	Path Forward	Comments on Transients
Fuel Salt			
Physical properties - Heat capacity of fuel salt [As a function of temperature, composition]	Fundamental to molten salt simulation, e.g. FoM1.	The properties of chloride salt fuels must be measured over the range of expected conditions. Properties of chloride salt fuels are very uncertain.	Range of conditions for which properties must be known is expanded. Has a potentially much larger impact on power/cooling mismatch events.
Physical properties - Thermal conductivity of fuel salt [As a function of temperature, composition]	Fundamental to molten salt simulation, e.g. FoM1, FoM2	The properties of chloride salt fuels must be measured over the range of expected conditions. Properties of chloride salt fuels are very uncertain.	Range of conditions for which properties must be known is expanded.
Physical properties - Viscosity of fuel salt [As a function of temperature, composition]	FoM1, FoM2, FoM3	The properties of chloride salt fuels must be measured over the range of expected conditions. Properties of chloride salt fuels are very uncertain.	Range of conditions for which properties must be known is expanded. Increased importance in natural circulation and timing of natural circulation.
Physical properties - Coefficient of expansion of fuel salt [As a function of temperature, composition]	Determines flow characteristics and neutronic behavior. FoM1, FoM2, FoM3, FoM4	The properties of chloride salt fuels must be measured over the range of expected conditions. Properties of chloride salt fuels have high uncertainty.	May be important in over-power transients and transients that require passive decay-heat removal. Impacts natural circulation and neutronics.
Physical properties - Optical properties of the fuel salt [Spectral dependence of optical absorption]	Affects thermal radiation heat transfer. FoM1.	Optical properties must be measured, including effects of fission product contamination.	Range of conditions for which optical properties must be known is expanded.

Phenomenon [Definition]	Impact	Path Forward	Comments on Transients
Heat transfer to core structure (convection and radiation) [Under forced/natural convection. Need to consider 'first wall' core structures]	Important for determining the heat load on 'first wall' core structures. Radiation component will be dependent on the optical characteristics of the salt fuel. FoM1.	Convective heat transfer is well understood, but radiation heat transfer is dependent on the optical properties of the salt fuel.	May be important due to impact on controlling heat release back to the fuel salt and controlling heat transfer during an event. Affects approach to limiting conditions for core structures.
Heat transfer to piping/vessel in primary circuit [Under forced/natural convection and radiation. Does not include heat exchanger]	Heat transfer, temperature limits, and plate-out on walls are a concern. FoM1, FoM6.	Convective heat transfer is well-understood, but radiation heat transfer is dependent on the optical properties of the salt fuel.	May be important due to impact on controlling heat release back to the fuel salt and controlling heat transfer during an event. Affects approach to limiting conditions for core structures and 'first walls'.
Heat transfer to heat exchanger [Under forced/natural convection. Dependent on plated-out materials]	Impacts all FoMs.	Heat transfer to the heat exchanger absent fouling is well-understood. Heat exchanger design will have an impact on heat transfer performance and prediction capability.	See "Primary Heat Exchanger" system below.
Fouling / Plating-Out [Precipitation and contaminants collecting on heat exchanger surfaces. Corrosion, fission products, and fissile material are the sources of fouling. Time, location, and operation dependent]	Increases the resistance to heat transfer, fluid flow. FoM1, FoM6.	Need to develop a predictive method to determine the rate of deposition, deposition composition, and impact on heat transfer coefficient. Chlorides tend to dissolve a larger amount of fission products if they are radiation stable.	May be important to over-cooling events in which fissile materials will plate-out at coldest locations (e.g. heat exchanger).

Phenomenon [Definition]	Impact	Path Forward	Comments on Transients
Form loss coefficients [Loss coefficients as a function of area ratio and Reynolds number]	Fundamental to molten salt simulation. Determines the flow. FoM3. May be less important due to lack of core structure in publicly available preliminary design information.	Design dependent. Form loss coefficients are generally well understood.	Potentially important to low and natural circulation flows.
Multi-dimensional flow. [Need for three-dimensional flow modelling within pool.]	Design detail dependent. Computational fluid dynamics likely because of lack of internal structures in core region. Affects all FoMs.	Design dependent.	Design dependent. Transient could increase asymmetry of flow.
Wall friction [Dependent on surface conditions, Reynolds Number]	Fundamental to molten salt simulation. Determines the flow. FoM3.	Need to know surface condition (roughness, plated-out material) as well as the shape of the passages.	Potentially important to low and natural circulation flows. Requires characterization over a larger range of Reynolds numbers.
Salt freezing [Temperature at which the salt solidifies. Dependent on composition]	Impact on steady state will be low unless part of the reactor design. Larger impact on transients. FoM6	The melting point is easy to measure, but is expected to be dependent on composition. Phase diagrams for chloride salt fuel are poorly understood.	May become important for over-cooling events.
Particulate formation [Result of conglomeration of quasi-Noble fission products]	Causes surface degradation due to abrasion. FoM3, FoM6.	Design particulate formation out of the system or implement mitigation systems. Path forward is to be determined due to number of unknowns.	May become important for over-cooling events.
Bubble distribution [Noncondensable gas bubbles, sparging gas, and fission product bubbles entrained in the fuel salt. Void fraction and bubble size distributions]	Design specific: FoM2, FoM4, FoM5.	Determined by experiment, dependent on the design. May require two-component models.	Voids within the salt, due to sparging, gas production, or entrainment of cover gas can affect reactivity.

Phenomenon [Definition]	Impact	Path Forward	Comments on Transients
Fuel salt volatility [Transport of fission products and fissile material through evaporative processes]	FoM1, FoM2, FoM4, FoM5	Requires experiments to determine volatility of fuel salts. Chloride salts tend to have higher volatility. Uncertainty is high.	Transients will drive more volatile material into the gas space. Volatility of the salt can result in transport of fission products and fissile material to the cover gas and cover gas system.
Radiation stability [Resistance of the fuel salt to radiolytic decomposition]	FoM4	May be important to chemical composition codes, but not to neutronic/thermal-fluid codes.	Transients may drive a larger radiolytic decomposition.
Molten salt break flow [Leak of a molten salt as a function of hole size and driving head, and its solidification and capability to plug a hold in the primary boundary]	FoM1, FoM3, FoM6.	May require experimental data to develop the applicable flow and solidification models. Foundry industry models may be extended.	Most applicable to transient conditions.
Fuel salt mixing in the core [Velocity distribution of the salt fuel in the core. May involve mixing of different streams.]	The core velocity distribution contributes to the core temperature distribution. FoM1, FoM3.	Detailed evaluation or nodalization to resolve temperature distribution.	Potentially important in transients. Must be able to calculate temperature distribution in the core.
Core Materials			
Physical properties. Thermal properties of core materials [Thermal properties as a function of temperature and irradiation. Includes mechanical support elements, control elements, and reflector]	Shutdown rod only present during shutdown. 'First wall' and reflector must also be considered. May need to consider liquid lead reflector. FoM1.	Material properties are generally well known.	No special consideration for transients.

Phenomenon [Definition]	Impact	Path Forward	Comments on Transients
Geometry [Physical dimensions and configuration of the core materials. Includes swelling and deformation]	Surface area and flow area changes are important for all FoMs. Also impacts neutronics due to changes in core neutron leakage. Affects all FoMs.	Geometry is dependent on design. Geometric changes must be taken into account.	Need assurance that transients do not cause adverse changes in geometry. Control rod movement may cause flow geometry change.
Direct energy deposition [Fraction of energy assumed to be deposited at site of core structures]	Impact is important to closest internals or structures. FoM1, FoM2.	Gamma energy is known fraction but location of deposition not known, but can be modeled.	May be important in over-power transients.
Bypass Flow [Fuel salt flow intended to cool the shield/reflector]	FoM1, FoM3. Must consider potential for blockage and associated consequences.	Design-specific information must be provided.	No special consideration for transients.
Vessel/Piping			
Physical properties. Piping and liner (if used) properties [Density, specific heat, and thermal conductivity of piping and liner materials]	Liner may or may not be part of the design. Affects stored energy of surrounding structures. Impacts FoM5.	Metal properties are generally well known or can be determined.	May impact stored energy during transients. Range of conditions for which properties must be known is expanded and time history may become important.
Piping/vessel failure modes induced by thermal and mechanical stresses in an accident (e.g. creep rupture)	Could require a guard vessel or guard piping. FoM1	Creep rupture parameters are generally known or can be determined.	Could initiate a compounding failure
Insulation properties [Resistance to heat transfer to containment environment]	Affects heat loss. FoM1	Material properties are generally well known. Design information on the insulation must be provided.	Potential influence on fuel salt solidification. Could represent an initiating event. Insulation properties are important to natural circulation.
Direct energy deposition [Fraction of energy assumed to be deposited in vessel and piping materials]	Need to know where energy is deposited. FoM1, FoM2. Also possible effect on maintenance operations. Impacts FoM5.	Gamma energy is known fraction but location of deposition not known, but can be modeled.	Similar importance to steady-state. Contribution from plated-out fission products may become significant.

Phenomenon [Definition]	Impact	Path Forward	Comments on Transients
Primary pumps			
Pump performance [Relationship between driving force, flow rate, and efficiency as a function of temperature and salt composition]	Pump working condition is included in the initial conditions in modeling for all events. FoM3.	Vendor supplied information	Will require coastdown characteristics.
Pump resistance or K factor [Pressure drop across pump]	Pump is an additional flow resistance when not working. Low impact on steady-state operation. FoM3.	Vendor supplied information	Will need to know a locked-rotor k factor and variation as a function of Re.
Gas entrainment in pump [Sweep-out of gas space by the pump into the fuel salt]	Impacts reactivity if gas is convected into the core. Higher flowrates for fast reactors may exacerbate the effect. FoM1, FoM2, FoM3, FoM4, FoM5.	Develop gas entrainment models and bounding analysis for normal operation based on vendor-supplied information. Design specific.	Not an issue for pump trip. May be important for pump overspeed transient.
Pump cavitation [Gas evolution at low pressures]	Impacts reactivity if gas is forced into the core. Degrades pump performance and lifetime. FoM1-5.	Develop appropriate flow models for cavitation.	Not an issue for pump trip. May be important to pump overspeed transient.
Primary heat exchanger			
Primary side convective heat transfer [Under forced/natural convection. Dependent on plated-out materials]	Impacts all FoMs.	Heat transfer to the heat exchanger absent fouling is well understood. However, high-performance heat exchangers may be required to deal with the high heat flux. Heat exchanger design will have an impact on heat transfer performance and prediction capability.	May be important in natural circulation. Highly dependent on event and design.

Phenomenon [Definition]	Impact	Path Forward	Comments on Transients
Primary side flow resistance [Combined wall and frictional drag across the primary side of the heat exchanger]	FoM1, FoM3.	Vendor-supplied information.	May be important in natural circulation. Highly dependent on event and design.
Secondary side convective heat transfer [Under forced/natural convection]	Impacts all FoMs.	Heat transfer to the heat exchanger absent fouling is well understood. However, high-performance heat exchangers may be required to deal with the high heat flux. Secondary-side fluid properties, will need to be determined. Heat exchanger design will have an impact on heat transfer performance and prediction capability.	Highly dependent on event and design.
Conduction through heat exchanger surfaces [Net resistance of heat exchange surface, including fouling layers. Conduction through the wall materials]	FoM1, FoM3.	Modeling of heat exchanger performance will need to account for surface and material properties.	May be important in natural circulation. Highly dependent on event and design.
Fouling and plate-out [Precipitation and contaminants collecting on heat exchanger surfaces. Corrosion, fission products, and fissile material are the sources of fouling. Time, location, and operation dependent]	Increases the resistance to heat transfer, fluid flow. FoM1, FoM3.	Need to develop a predictive method to determine the rate of deposition, deposition composition, and impact on heat transfer coefficient.	Highly dependent on event and design. Will be treated as additional heat transfer resistance during transients. Additional plate-out during an over-cooling transient has the potential for actinide deposition.

4.4 Solid-Fuel MSRs

The primary intent of this pre-PIRT activity was to consider the phenomena that need to be modeled to simulate liquid-fuel MSRs. Recent PIRTs exist for both neutronics phenomena [4-8] and thermal-hydraulics phenomena [4-9] for solid-fuel MSRs. Furthermore, a recent workshop [4-10] building on those PIRTs, has gone further to identify the technology gaps that exist in the modeling of solid-fuel MSRs.

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5 SUMMARY AND RECOMMENDATIONS

5.1 Modeling/Simulation Needs

5.1.1 Neutronics

Neutronics analysis for steady state, operational transients, and accidents in MSRs requires addressing unique reactor physics challenges with key interfaces and phenomenological coupling to both thermal-hydraulic and inventory control and distribution phenomena. Two main challenges are introduced with liquid fuel: delayed neutron precursor motion, and strong coupling to salt composition. Hence, it is necessary to take into account the movement of delayed neutron precursors into and out of the core, and the transit times of the fuel, fission products, and transmutation and chemistry products through the primary system.

It has been demonstrated previously that the impact of the movement of delayed neutron precursors into and out of the core, and the transit times of the salt components through the primary system can be conservatively bounded. In support of the Molten Salt Reactor Experiment (MSRE), a relatively simple model was used to show that MSRE dynamics could be conservatively bounded [5-1]. That dynamic model predicted that the reactor was stable and controllable over its entire power range. An extensive experimental program validated that model and the inherent safety characteristics of that small experimental reactor [5-2]. The modeling and simulation fidelity required for motion of delayed neutron precursors and other salt components may be dependent on reactor design, licensing approach (e.g. licensing a test reactor versus a commercial demonstration reactor), and the magnitude of the source term.

The salt composition in the core defines neutronic properties and the composition throughout the primary system defines accident source terms. Identification of isotopes to track in depletion simulations is related to salt composition and chemistry, and is closely coupled to the operational history. Operational history impact depletion accounting for the presence of control rods or other spectrum changing asymmetries within the core, including power operation history. This unique coupling of neutronics, chemistry, and inventory control is a novel aspect of molten salt reactor simulation.

MSR concepts could operate in thermal, intermediate, and fast neutron spectrum configurations. This assumes the definition of a system spectrum as having the majority of fissions occurring at thermal (less than 1.0 eV), intermediate (greater than 1.0 eV but less than 100 keV), or fast (greater than 100 keV) energies. Consequently, MSRs fueled with a mixture of fertile thorium (^{232}Th) and recovered uranium (mostly ^{233}U, ^{234}U, and ^{235}U) are capable of operating in breakeven or breeding fuel cycles in a thermal or intermediate spectrum.

This pre-PIRT effort considered both thermal spectrum and fast spectrum MSR concepts. Thermal spectrum concepts typically use fluoride salts, and fast spectrum concepts use fluoride or chloride salts. The neutron flux spectrum of an MSR can vary between a thermal spectrum and a very fast spectrum. Three examples of neutron flux spectra of MSRs are shown in Figure 5-1; a thermal solid-fuel design (FHR) [5-3], a fast spectrum molten chloride fast reactor (MCFR) [5-4] and an intermediate spectrum liquid-fueled thorium MSR (IS_MSR) [5-5]. The spectra for different MSR concepts are compared with those of a generic light water reactor (LWR) and sodium-cooled fast reactor (SFR). The objective of this discussion and figure is to show the diverse array of neutronic characteristics of potential MSR concepts.

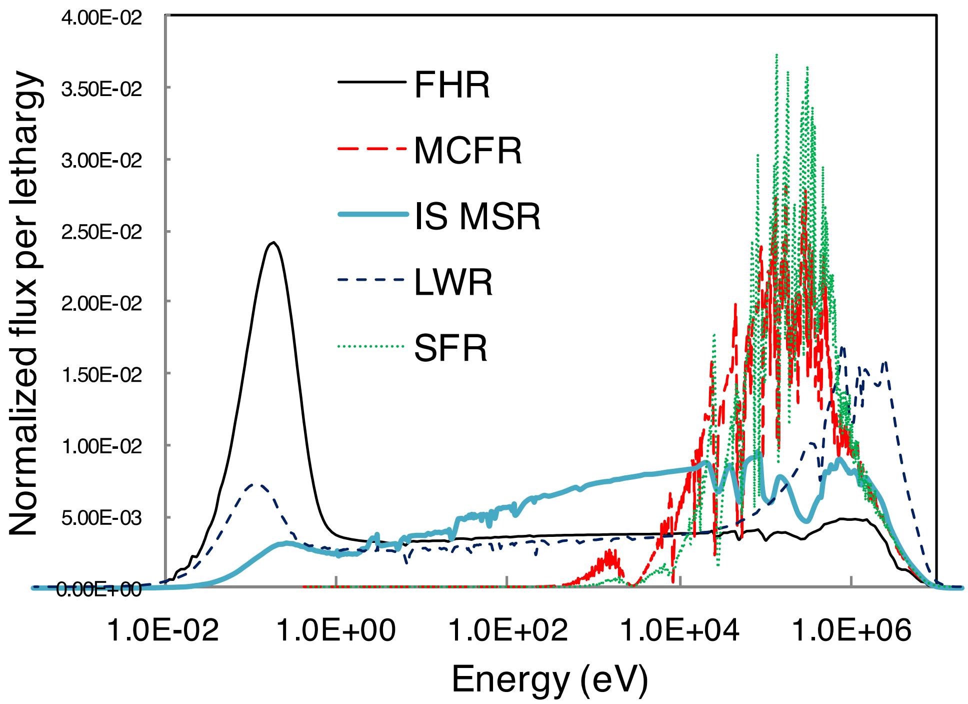

Figure 5-1 Neutron Flux Spectrum in Molten Salt and Other Reactor Designs

For both thermal and fast spectrum MSRs, the transmutation and inventory of salt constituents that are parasitic absorbers like ^{6}Li (for thermal MSRs with salts containing lithium) or ^{35}Cl (for chloride fueled fast reactors) has a major impact on reactor neutronics. This directly impacts all neutronics FoMs. In particular, ^{6}Li has a large absorption cross-section and is the major contributor to production of tritium in thermal spectrum MSRs. For thermal MSRs, the ^{6}Li(n,t)^{4}He cross section and ^{9}Be(n,α)^{6}Li cross sections are well known. Typically, these reactions happen on time scales that are not important for reactor transients, but the inventory will evolve over the lifetime of the reactor. As irradiated salt constituents are replenished with fresh inventories the impact will also evolve. In addition to impacting the neutronics, the tritium source term is needed for accident consequence analysis.

Similarly, <u>neutron absorption in fuel salt</u>, including fission products, will have a significant impact on MSR neutronics for both fast and thermal systems. Hence, absorption cross-sections for the fission products and constituents of the fuel salt are important. Transmutation of some chlorine isotopes can lead to the production of sulfur in the reactor. This is highly coupled to inventory control phenomena, and impacts the source term during consequence analysis. Additionally, this has a direct impact on the fuel salt and coolant chemistry during operation, and interfaces directly with the inventory control and distribution phenomena. Fission products will have much less of an impact on a fast spectrum system than a thermal spectrum system. Neutron cross sections for minor actinides have a high uncertainty, but the impact may be low.

The moderation and thermalization of neutrons by the fuel salt occurs, but is expected to have a relatively small impact on thermal MSR neutronics. However, moderation and thermalization of neutrons in graphite will have major impacts on neutronics of some thermal MSR designs. Similarly, for those designs that use alternative moderators, such as ZrH, neutron moderation will have significant impacts on the reactor physics characteristics of the system. These effects are well understood and have quantified uncertainties.

Another challenge is photoneutron production from beryllium and fluorine, including neutron production in beryllium from (γ,n), (α,n) and (n,2n) reactions. These delayed neutron data may be more important for transient analysis than for steady state. The impact may be small, but the uncertainties are high.

Reactivity control through absorption of neutrons in control rod materials and/or the displacement of salt fuel is another unique aspect of reactor physics modeling of MSRs. As with any reactor, measurements must be made to confirm predictions of control rod worth. Calculations have to account for the in-core residence time and the appropriate depletion chains for control materials. The importance of these phenomena is highly design dependent, especially since some MSR designs would be operated with low excess reactivity (and less need for control rod operation), due to the potential for online refueling.

5.1.2 **Thermal-Hydraulic Analysis**

Thermal-hydraulic analysis of molten salt reactors has several unique and challenging features in comparison to other reactor systems. Thermal-hydraulics and neutronics are expected to be tightly coupled, and phenomena for each technical discipline will affect the other. The pre-PIRT panel has identified several phenomena important to thermal-hydraulics in Chapter 4. Table 4-4 lists the phenomena for thermal-spectrum fluoride salt reactors, and Table 4-8 those for fast-spectrum chloride salt systems. In general, most of the phenomena important to fluoride salts are also important to chloride salts. This section summarizes and categorizes these phenomena into several areas, and identifies some of the major challenges to modeling and simulation of MSR thermal-hydraulics.

Compared to light water reactors, the lack of high pressure operation, energetic break flow, depressurization, quench front tracking, and two-phase flow may simplify many aspects of a MSR analysis. Molten salt reactors however, have unique aspects that result in the consideration of new phenomena. These must be accounted for in the simulations performed by an applicant, as well as by the confirmatory analyses by the NRC.

For MSRs, one of the important issues is that of physical properties. This was found to be important for both fluoride salts and chloride salts. Physical properties for MSRs encompass several individual thermophysical properties, including thermal conductivity, viscosity, specific heat, density, and optical properties such as emissivity and transmissivity. Also included as part of physical properties are thermodynamic properties including the boiling and melting points, enthalpy, phase equilibria, and volatility of the salt and other components of the coolant. In general, physical properties are vital to accurate simulation of fluid flow and heat transfer, and thus are considered a high priority item. Accurate knowledge of these properties must cover the full range of conditions expected during both normal operation and in accident scenarios. While boiling of a molten salt is not expected, should there be scenarios in which boiling becomes a possibility it will be necessary to determine physical properties such as latent heat of vaporization and vapor density. Fluoride salts have a more established database and thus a smaller uncertainty in physical properties than chloride salts. However, improvement in the database and means to estimate thermophysical properties will likely be necessary for both fluid systems.

Convective heat transfer was identified as an important process. Here, the concern is the uncertainty associated with heat transfer in a molten salt. The physics of convective heat transfer in fluids is generally well understood. However, because geometry and physical properties are important in convective heat transfer, and the database for molten salts is limited, this is a physical process that is expected to require some attention.   Heat exchanger design will depend in part on simulation of convective heat transfer processes. In particular, information to inform the selection of appropriate and accurate correlations for forced and natural convection in a molten salt system will be needed.

Similar to convective heat transfer, primary system flow resistances were identified as processes and parameters of importance in an MSR. This includes frictional and form loss from structures in contact with the molten salt. Accurate modeling of flow resistances is necessary when simulating natural circulation, which is expected to be a dominant mode of transport in many accident scenarios. Closely related to primary system flow resistance is multi-dimensional flow in designs with “open pools” or those lacking a significant number of internal structures. In this case, the resistance is due to viscous dissipation and recirculation within the flow. For those designs with large pools it will likely be necessary to incorporate computational fluid dynamics into the analysis method.

Structural material performance and behavior is a category of physical processes that are expected to be important in thermal-hydraulic analysis. This includes the swelling of material within the system and thermal expansion. These processes affect the geometry and thus the flow areas and bypass flows. Changes in geometry and expansion of the core can also affect reactivity. Direct energy deposition in structures can affect the temperature distribution in the structures and coolant. For fuel in salt concepts, an increased emphasis will be placed on the performance of barriers to the release of radioactive material outside the fuel in contrast to solid-fuel reactors in which the first barrier to release of radioactive material is the matrix and cladding of the fuel itself. Thus, a thermal-hydraulic confirmatory analysis tool will likely be used to analyze the potential for failure of the primary system, such as by thermal creep.

The salt chemical composition represents a technical issue that depends on numerous physical processes. In a liquid fuel MSR the molten salt will eventually include an inventory of fission products which will decay depending on the particular isotope. As the fission products are generated and decay, the chemical composition of the fuel salt will change. Some products may be insoluble creating the potential for plate-out of those materials on surfaces. Plate-out on heat transfer surfaces may result in an additional thermal resistance to heat transfer that will have to be taken into account. The potential also exists for there to be chemical reactions between some chemical species in the salt as well as with structural materials. Corrosion products and their impact on the salt and reactor materials will need to be assessed, to the extent that they are not minimized by chemistry control and material selection.

In a liquid-fuel MSR combined with a fuel cycle facility, the salt chemical composition may become complex as fluid is withdrawn and added to the primary system. Combined with the other processes that can change salt composition, depletion, fission product decay, chemical reaction, solubility, etc., the chemical environment of an MSR may be dynamic and dependent on plant operation. Section 5.2 discusses simulation of the MSR inventory.

An issue that was identified as specific to thermal spectrum fluoride salt MSRs is that of tritium production and transport. Tritium is produced by neutron absorption in ^{6}Li, which has a very large absorption cross-section and by beryllium. While most designs intend to use enriched lithium, in which ^{6}Li is replaced by ^{7}Li to reduce tritium production, non-trivial amounts of tritium may be generated. The total production rate, and its transport to system boundaries where tritium can be captured is a concern and will need to be addressed. The hold-up of tritium in graphite and release rates during high temperature transients may contribute to the source term. This tritium would enter the fuel salt and be transferred to the system boundaries. Knowledge of the tritium retention and release mechanisms are needed.

Processes involving gas entrainment and transport were identified as potentially important in both fluoride and chloride fuel salts due to their effect on multiple FoMs. These processes include the separation of fission gases from the liquid, and the entrainment of a cover gas on the surface of the liquid pool. Depending on design of the system, pumps using a cover gas could also be a source of entrained bubbles. Sparging, which may be useful in removing contaminants through injection of helium or other inert gas would result in voids that would need to be simulated due to their effect on reactivity. Tritium and any gas produced by radiolysis would be important considerations if produced in quantities sufficient to generate voids in the primary coolant.

5.2 Inventory Control and Distribution

In the previous sections, several processes were identified that involve the chemical inventory of a molten fuel salt reactor. Composition of the salt and the distribution of some chemical species within the system can have important effects on accident scenarios and their results. Some liquid-fuel MSRs are expected to be integral plants that contain a chemical fuel processing plant co-located with the nuclear reactor facility. Maintaining inventory control at the site will be challenging, as fissile material and fission products will be repeatedly transferred. Determination of the inventory is important as an initial boundary condition to accident scenarios involving the reactor facility. This also means that accidents other than those needing reactor simulation (i.e., in the fuel processing plant) will be an important safety concern.

A major recommendation of this study is that modeling and simulation of MSRs will require development of computational tool(s) capable of tracking chemical inventories of constituents throughout the primary loop of the reactor facility. Such a tool is not a vital part of water reactor safety analysis since the coolant is a single component (either light or heavy water) with dilute concentrations of other species such as boron or lithium. Thus, an inventory control and evaluation tool is a unique feature necessary for liquid-fuel reactors. (The issue may be relevant to solid-fuel MSRs but was not a consideration in this pre-PIRT.) A comprehensive evaluation of fuel salt composition will likely require the modeling of salt chemistry, thermodynamics, mass transport, and addition and removal of chemical species. Fission and transmutation products will be generated in the salt and will form a variety of chemical species. The phase behavior of these species is complex, and depends on the specific design, particular fuel salt, and plant operation.

Key issues related to inventory control and distribution include fission product generation, transmutation of isotopes of the salts (e.g., ^{6}Li in a fluoride salt reactor or ^{35}Cl in a chloride salt reactor), corrosion, particle agglomeration, filtering, plate-out of insoluble components, chemistry control, fuel salt processing, and fission product separation (active or passive) including clean up by gas sparging. Each of these physical behaviors and related systems depend on the solubility limits of the relevant fuel, and fission product and transmutation product constituents within the salt. Additionally, cover gas may become entrained in the fuel salt itself and may need to be tracked. Alternatively, the fuel salt may become entrained in the cover gas and transported out of the primary system to the fission gas storage system.

For some molten salt fuel compositions and mixtures, there is limited knowledge about phase diagrams and potential radiolysis. Relatively sparse data exist relative to the 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. There is a need to establish phase diagrams and radiation stability data for some candidate fuel salts, in particular with chloride salts and those containing fission products. Fundamental thermodynamic data, such as Gibbs free energies and interatomic potentials, are needed for these mixtures to develop these phase diagrams. There is also a strongly related need for a fuel salt irradiation program to gather the required data regarding radiolysis.

Many salt constituents, such as ^{6}Li, are relatively strong neutron absorbers and will transmute. This will mean that the isotopic and chemical inventory of the salt constituents themselves will be changing with time on stream in the primary loop.

Corrosion is a possible concern, and may need to be simulated as part of a system inventory calculation. Some fuel salts have been found to be corrosive, although use of a nickel-based alloy such as Hasteloy N has been found to be corrosion resistant. The need for accounting for corrosion products in the system inventory will eventually depend on the salt and components in contact with the salt. The MSRE experience [5-6] provided some information on corrosion and its control. In order to limit corrosion or the potential for oxide precipitation, chemistry control is essential including redox potential and the concentration of dissolved oxide contaminant.

5.3 Experimental Gaps

Molten fuel salt reactors would have significantly different neutronic, thermal-fluid and chemical behavior than existing reactors and may require a wide range of fundamental experiments to characterize their performance and safety. To date there have only been two domestic MSR test reactors, the Molten Salt Reactor Experiment (MSRE) [5-7] and the Aircraft Reactor Experiments (ARE) [5-8]. Both of these experiments used the fuel dissolved in the heat transfer salt. There has also been a number of separate effects experiments focused on understanding fundamental issues mainly focused on fluoride salts and to a much lesser extent chloride salts. The majority of these were conducted at Oak Ridge National Laboratory (ORNL) during the period of MSRE operation and are fairly well documented. Recently, there have been a handful of other separate effects experiments performed at U.S. national laboratories and abroad at other laboratories and universities. There remain several areas that need further investigation and confirmation in order to have a fundamental grasp of the thermal-hydraulic and safety performance of an MSR. New flow loops and integral test facilities utilizing molten salts will likely be necessary to develop models and correlations, and to assess code performance.

There is a clear need for fundamental thermophysical properties measurements and quantification of uncertainties. It has been suggested that for the FLiBe and FLiNaK salts, properties are known to within about 10% [5-9]. This may not be acceptable for accurate design analysis or licensing of an MSR. Properties can vary considerably in pure fluids containing small amounts of a contaminant. Thus, it may be necessary to expand the property database to include a consistent set of thermophysical properties for fuel salts containing additional chemical species dissolved into them. For salts other than FLiBe and FLiNaK, the database is relatively weak and a comprehensive experimental program is necessary to develop a reliable database of properties.

For fast spectrum chloride salts, there is a need for high flux radiation stability tests to determine if radiolysis effects are significant and to determine the extent and distribution of fission gas products. The radiolysis of the salts could affect the composition of the salts and lead to formation of corrosive gaseous products such as chlorine gas. The rate of radiolysis and recombination is currently not known and needs experimental evaluation.

Unique thermal hydraulic issues that require separate effects and integral tests include the freezing point as a function of the dissolved constituents in the salt, entrainment of gases (including cover gas), and the transport throughout and release of noble gases and tritium from the plant. Models for gas transport, including for tritium, must be developed and validated using appropriate testing. Tritium diffusion models need to be developed, including those that consider plate-out behavior. Thermal stratification models for fluids with high Prandtl number are also necessary to understand the behavior of molten salt reactors. Data on system and component performance, for example pump performance and cavitation data, are needed for both thermal and fast spectrum MSRs.

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This study has identified key phenomena that are vital for the modeling and simulation of molten salt reactors, with a focus on liquid-fueled reactors. The large number of MSR concepts and system designs means that there is wide variation in the potential predictive modeling needs. The phenomena identified in this report are design independent, because none of the designs have progressed to the needed level of maturity to conduct a full PIRT activity as of the publication of this report.

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