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

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

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

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

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

ABSTRACT

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

KEYWORDS
Liquid-fuel, molten-salt, thermal-hydraulics modeling.

1. INTRODUCTION

1.1 Background

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

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

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

1.2 Objectives

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

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

2. METHODOLOGY

In assessing the adequacy of computer codes to address accident phenomena and to identify areas of needed improvement, the NRC has frequently followed a process known as Code, Scaling, Applicability and Uncertainty (CSAU). CSAU is a structured process that helps define code capability and ensures that physical processes important to an accident scenario are properly taken into account. One of the first steps of CSAU involves development of a Phenomena Identification and Ranking Table (PIRT) [7]. The PIRT process involves a review of the design for particular events and identification of the physical phenomena expected to be most dominant. In development of the PIRT a group of technical experts identifies the phenomena and ranks the state of knowledge of each phenomenon and its importance to safety-related consequences. The phenomena with high importance and low knowledge level then become a priority for future research, which may be analytical or experimental.

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

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

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

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

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

3. MOLTEN SALT REACTOR DESIGN

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

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[a] Panel members are given in the Appendix.

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

4. SIMULATION SCENARIOS

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

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

4.1 Normal Operation

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

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

4.2 Reactivity Events

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

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

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

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

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

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

4.3 Increase/Decrease of Temperature

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

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

5. THERMAL-HYDRAULIC PHENOMENA FOR MSRS

5.1 Figures-of-Merit

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

Before generating these tables, as part of the pre-PIRT process the panel chose the FoMs in Table I which are applicable to both thermal and fast spectrum designs. These FoMs are intended to reflect the importance and impact of specific phenomena.

Table I Figures-of-Merit for MSR Thermal-Hydraulics

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.

The tables of physical processes (phenomena) were generated separately for thermal and fast spectrum designs [5]. The context was the ability to model steady state conditions and then, as an ancillary activity, for the analysis of transient scenarios. The results are given below according to whether they are physical properties, or heat transfer or fluid flow phenomena or whether they relate to the transport of gases or solids. They are generally applicable to both thermal and fast spectrum reactors; however, the relative importance to safety analysis of the phenomena and their state-of-knowledge are different. In general the phenomena that must be modeled to simulate fast spectrum reactor behavior are less well-known than for thermal reactors because the fast reactor designs have received less attention by design organizations in the past.

5.2 Physical Properties

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 and transmutation products, 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 for the fuel salt are heat capacity, thermal conductivity, viscosity, and the coefficient of thermal expansion. Heat capacity and thermal conductivity directly impact the temperature of the fuel salt (FoM1) and through neutronic feedback, power (FoM2). The properties of pure fluoride salts are generally well-known with thermal conductivity having a greater uncertainty than heat capacity. Significant measurements are being done at Karlsruhe Institute of Technology (e.g., [14]). The viscosity of the fuel salt also impacts temperature and hence, FoM1 and FoM2. Obviously, it also impacts FoM3. Although some measurements have been made, it is clear that additional measurements of viscosity will be needed to cover variations in salt composition and the range of conditions during transients/accidents. The coefficient of thermal expansion of the fuel salt helps to determine flow characteristics (FoM3) and is particularly important in determining natural circulation conditions. It directly determines fuel salt density and hence FoM4. Since flow affects temperature, it has an impact on FoM1 and FoM2.

Surface tension is another property of potential importance for bubble transport and hence, directly impacts FoM5. Optical properties of the fuel salt may also be needed but were not discussed in depth. In general, the physical properties of the fluoride salts are known with reasonable accuracy, while chloride salt properties are not well known.

The heat capacity, thermal conductivity and coefficient of expansion of core materials such as for mechanical support, or as moderators or control elements have varying influence on FoMs. The properties determine temperature and/or density and may impact FoM6; for moderators they will impact FoM2. In general these properties are well known.

The similar properties for vessel and piping (and possibly liners) materials may impact FoM5 and FoM6 since these FoMs are functions of temperature. This also relates to knowing the failure modes for these materials and those involve aging effects, corrosion, thermal and mechanical stresses and radiation damage. Although properties of metals are generally well known, all the alloys that will be used were not known by the panel and there may be uncertainties due to the varied contributors to failure modes.

Insulating materials will likely be used and they will impact FoM1 and in a transient may influence natural circulation (FoM3). Properties are generally 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. Phase diagrams of some salts are unknown in the presence of fission products, transmutation products, and impurities. Although the Molten Salt Reactor Experiment experience at Oak Ridge National Laboratory [15] 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.

5.3 Heat Transfer Properties

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 discussed above.

Correlations for Heat Transfer between Fluid and Structures: This is relevant for the salt in contact with core structures and piping/vessel, and in the primary heat exchanger(s), both on the primary and secondary sides. It impacts all of the FoMs to varying degrees. 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. The effects are understood better for forced convection than for natural circulation and the presence of fouling will complicate understanding the impact.

Direct Energy Deposition: This phenomenon is more directly related to radiation transport rather than a heat transfer property but is relevant to the calculation of fluid and structure temperatures (FoM1) (and is also relevant to FoM5). The fraction of energy assumed to be deposited in core materials and vessel/piping can be calculated using neutronic methods assuming the power distribution and the location of fission products are known.

5.4 Flow Related Phenomena

Flow is analyzed in reactors using methods that assess fluid behavior satisfying conservation laws (mass, energy and momentum) and constitutive relationships for multi-component flow. Typically, it is necessary to couple the flow 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. All flow properties impact FoM3 and may have a bearing on all the others.

Both forced flow and natural circulation must be considered. The former 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 acceleration and deceleration associated with changes in flow geometry. Natural circulation 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.

Form Losses: This refers to the resistance to flow resulting from changes in geometry (expansion, contraction, and 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 and can be obtained once designs are specified. Although form losses can be estimated based on generic correlations, in practice it may be necessary to determine these losses empirically based on scaled models of the actual system design.

Frictional Losses: This refers to the resistance to flow associated with the frictional interaction between the fluid and the structure. Frictional losses are well studied for different flow regimes. Coefficients are tabulated as a function of Reynolds number and surface roughness. Deposition on surfaces (and corrosion) prior to or during the course of an accident changes the magnitude of the frictional loss coefficient and this may be particularly important in molten salt reactors.

Flow Regimes: Flow in pipes is characterized as laminar, turbulent or transitional, which affects 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.

Mixing: The calculation of mixing in the vessel and the need for three-dimensional models may become important depending on the geometry of the system and any inlets/outlets that may be present. At this time it is not clear what the impact is on the FoMs. Computational fluid dynamics would be one way of treating the issue if it is important (an example is thermal striping in the upper plenum if channels are used in the core).

Primary Pump Performance: There are several phenomena that need modeling. The most basic is the relationship between the driving force, flow rate, and efficiency as a function of temperature and salt composition. It is assumed that this is known by virtue of a vendor's specifications. Pump resistance or K factor (pressure drop across the pump) becomes important during transients when the pump is not operating and again is vendor supplied. Gas entrainment (sweep-out of gas space) and pump cavitation (gas evolution leading to vibrations) impact reactivity if the gas is forced into the core and models may need to be developed to simulate pump overspeed transients.

5.5 Phenomena Related to Solids and Gases

Transport of Gases: Gases become important safety issues (FoM5) in liquid-fuel MSRs because a) if bubbles collapse there can be reactivity additions and b) the containment of radioactive gases (fission product noble gases and tritium) can be particularly challenging since they are released directly to the liquid fuel salt. Tritium production and transport is a potential issue for both normal operation and accidents. Tritium produced during normal operation can be absorbed in graphite and then released in accidents. There are several modeling aspects. The entrainment of cover gas needs to be determined and depends on design. The volatility of the fuel salt, the uptake of tritium by graphite in the core and the diffusion of tritium into the secondary system through the heat exchanger may need to be measured and taken into account in simulations. Lastly, two-fluid models may be needed in many simulations.

Potential for Solids: It has been stated above that heat transfer and fluid dynamics are impacted by the presence of corrosion or plate-out on surfaces. Hence, the fouling of the fuel salt is very important (albeit not the function of the simulations of concern herein). This fouling can also lead to the presence of solids within the fuel salt (note FoM6). Another aspect of this is particle formation as the result of the conglomeration of quasi-noble fission products, which can then lead to surface degradation due to abrasion. A solid that might need to be modeled in the tools of interest is the result of the freezing of the fuel salt under over-cooling accident conditions.

6.0 SUMMARY AND CONCLUSIONS

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

Thermal-hydraulic analysis of liquid-fuel molten salt reactors has several unique and challenging features in comparison to some other reactor systems. For example, thermal-hydraulics and neutronics are expected to be tightly coupled, and the continuous tracking of composition changes may be important in some designs. The focus of this paper is with fluoride salts as those important phenomena are in general also important to chloride salts.

<u>Physical properties</u> are important for both fluoride salts and chloride salts. The panel focused on the following thermophysical properties: thermal conductivity, viscosity, specific heat, density, and optical properties. Properties that may also be important are thermodynamic properties like the boiling and melting points, enthalpy, phase equilibria, and volatility of the components of the molten salt. Physical properties are vital to accurate simulation of fluid flow and heat transfer, and thus are considered high priority. 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. 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. Information to inform the selection of appropriate and accurate correlations for forced and natural convection in a molten salt system will be needed.

Primary system flow resistances were identified as processes and parameters of importance. 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.

Generation of gas via transmutation, radiolysis, chemical reaction, or entrainment of a cover gas could lead to the need to model gas transport through the primary system. The presence of gas impacts many physical properties. To understand how that gas presents itself requires understanding the separation of fission gases from the liquid, and the entrainment of a cover gas at the surface of the liquid. 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.

Structural material performance and related physical processes can impact thermal-hydraulic analysis. For example, the swelling of material within the system and thermal expansion affect the geometry and thus flow areas and bypass flows (and possibly affect reactivity as well). Direct energy deposition in structures can affect the temperature distribution in the structures and coolant. The limiting conditions within these MSRs may be material performance as it relates to the prevention of the release of radioactive material. 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 composition of the molten salt is a factor in determining not only thermal-hydraulic behavior but also neutronics and the potential for corrosion. As fission products are generated and decay, composition changes. Radiolysis and transmutation are important, for example in keeping track of gases and actinides. Some elements being added to the mix may be insoluble creating the potential for plate-out on surfaces or particle agglomeration. Plate-out on heat transfer surfaces may result in an additional thermal resistance. 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. If there is on-site fuel processing then the salt composition is changing as certain products are removed (e.g., gaseous fission products and/or actinides) and added (e.g., fissile and fertile material and material for chemistry control). These considerations lead to the conclusion that simulation of MSRs will require development of computational tools capable of tracking the composition of the molten salt.

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

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APPENDIX
MEMBERS OF THE PRE-PIRT PANEL

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

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

Mark Anderson
University of Wisconsin
Madison, Wisconsin 53706

Nicholas Brown
Pennsylvania State University
University Park, PA 16802

Richard Denning
Independent Consultant
Columbus, Ohio 43220

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

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

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

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

Xiaodong Sun
University of Michigan
Ann Arbor, Michigan