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Identification and Resolution of Gaps in Mechanistic Source Term and Consequence Analysis Modeling for Molten Salt Reactors Salt Spill Scenarios

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ABSTRACT

This report represents an assessment of the gaps in Mechanistic Source Term (MST) and consequence assessment modeling for Molten Salt Reactors (MSRs). The current capabilities for MELCOR and the MELCOR Accident Code System (MACCS) are discussed, along with updates needed in order to address specific needs for MSRs. A test plan developed by Argonne National Laboratories is discussed as addressing some of these gaps, while some will require additional attention. Further recommendations are made on addressing these gaps. This report satisfies the DOE NE Milestone M2RD-21SN0601061 to leverage MELCOR and MACCS to identify parameters of importance for source term assessments for salt spill experiments.

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CONTENTS

Abstract 3
CONTENTS 5
LIST OF FIGURES 7
LIST OF TABLES 7
Acronyms and Definitions 8
1. Introduction 10
 1.1. Executive Summary 10
2. Overview of Molten Salt Reactors 12
 2.1. Liquid-fueled Molten Salt Reactors 12
 2.2. Solid-fueled Molten Salt Reactors 13
3. Risk Assessment and Licensing for Molten Salt Reactors 15
 3.1. Background on Risk Assessment Activities 15
  3.1.1. Industry and Regulatory Activities for Technology-Inclusive, Risk-Informed, Performance-Based Processes 15
  3.1.2. Risk Assessment Attributes 15
 3.2. Generic MSR Risk Assessment 16
  3.2.1. Licensing Basis Event Selection 16
  3.2.2. Licensing Basis Event Evaluation 19
 3.3. Risk-Informed Insights 20
4. Mechanistic Source Term Modeling 22
 4.1. MELCOR 23
  4.1.1. FLiBe EOS 23
  4.1.2. Circulating Fuel Point Reactor Kinetics Equations 27
  4.1.3. Liquid-Phase Fission Product Chemistry and Transport Model 28
  4.1.4. Physics-Based Melt Spreading 28
  4.1.5. Brief Overview of Relevant MELCOR Code Packages 29
 4.2. Data Needs for Mechanistic Source Term Modeling 30
  4.2.1. Salt Spill Scenario: MELCOR Models/Capabilities and Data Needs 31
  4.2.2. Other Scenarios: MELCOR Models/Capabilities and Data Needs 33
5. Consequence Analysis Modeling 34
 5.1. MACCS Accident Consequence Code System (MACCS) 34
 5.2. Data Needs for Molten Salt Reactors 35

5.2.1. Released Radionuclides and Associated Chemical Forms 35
5.2.2. Chemical Forms and Unique Deposition Behavior 38
5.2.3. Off-Site Decontamination Methods 38
5.2.4. Near-Field Modeling 39
6. Molten Salt Spill Experiments 40
6.1. Test Plan from Argonne National Laboratories 40
6.2. Data needs of Importance for Mechanistic Source Term and Consequence Analysis Modeling 41
6.3. Recommendation Gap Closure 43
7. Summary 45
References 46
Distribution 48

LIST OF FIGURES

Figure 2-1: Diagram of a liquid-fueled Molten Salt Reactor developed as part of the Generation IV International Forum 12
Figure 2-2: Mk1 PB-FHR Schematic [3] 13
Figure 3-1. Liquid-fueled MSR safety function diagram [1] 17
Figure 3-2. Liquid-fueled MSR functional event tree. 18
Figure 4-1: *Li-BeF2 density curves at saturation* 24
Figure 4-2. Viscosity curve for Lif-BeF2 24
Figure 4-3. Vapor specific volume at saturation 25
Figure 4-4. Saturation curve for LiF-BeF2 25
Figure 4-5. Coefficient of thermal expansion for LiF-BeF2 26
Figure 4-6. Thermal conductivity calculated for LiF-BeF2 26
Figure 6-1: Argonne National Lab Salt Spill Experimental Setup [14] 40
Figure 6-2: Radionuclide vapors and aerosols 42
Figure 6-3: Recommended Pathway for Gap Closure 43

LIST OF TABLES

Table 5-1: Recommended additional nuclides for inclusion in off-site consequence analysis for fluoride salt MSRs, showing corresponding chemical group in MACCS [11] 35
Table 5-2: Recommended additional nuclides for inclusion in off-site consequence analysis for chloride salt MSRs, showing corresponding chemical group in MACCS [11] 36
Table 5-3: Recommended additional nuclides for inclusion in off-site consequence analysis for solid-fueled MSRs, showing corresponding chemical group in MACCS [11] 37
Table 6-1: Data needs for volatile radionuclides 42
Email—Internal 48
Email—External 48

ACRONYMS AND DEFINITIONS

Abbreviation	Definition
ANL	Argonne National Laboratories
CVH	Control Volume Hydrodynamics
DCH	Decay Heat
DID	Defense-in-depth
DOE	Department of Energy
EOS	Equation-of-state
EPZ	Emergency Planning Zone
ES	End State
FHR	Fluoride-Salt-Cooled High Temperature Reactor
FL	Flow Path
FMEA	Failure Mode and Effects Analysis
HAZOP	HAZard and OPerability study
HS	Heat Structure
HTGR	High Temperature Gas Reactor
HYSPLIT	Hybrid Single-Particle Lagrangian Integrated Trajectory
LBE	Licensing Basis Event
LMP	Licensing Modernization Project
LWR	Light Water Reactor
MACCS	MELCOR Accident Consequence Code System
MSM	Molten Salt Model
MST	Mechanistic Source Term
MSR	Molten Salt Reactor
NEI	Nuclear Energy Institute
NOAA	National Oceanic and Atmospheric Administration
NRC	Nuclear Regulatory Commission
PB-FHR	Pebble Bed Fluoride-Salt-Cooled High Temperature Reactor
PHA	Process Hazard Analysis
PRA	Probabilistic Risk Assessment
SAMA	Severe Accident Mitigation Alternatives
SAMDA	Severe Accident Mitigation Design Alternatives
SBO	Station Black Out
SNL	Sandia National Laboratories

Abbreviation	Definition
SSC	Structures, systems, and components
SOARCA	State-of-the-Art Reactor Consequence Analysis
TI-RIPB	Technology-Inclusive, Risk-Informed, Performance-Based
TRISO	Tri-structural isotropic

1. INTRODUCTION

1.1. Executive Summary

As Molten Salt Reactor (MSR) designs are maturing and their designers are embarking upon the licensing process within the United States and internationally, it is necessary to quantitatively characterize both the Mechanistic Source Term (MST) and associated consequences for MSR accident scenarios. This report discusses the need for enhanced MST and consequence analysis capabilities specific to MSRs to support reactor licensing efforts.

In regards to the Technology-Inclusive, Risk-Informed, Performance-Based (TI-RIPB) Licensing Modernization Project (LMP), the report highlights three risk-informed insights specific to MSR accident analysis and licensing applications:

- Salt spill and splash modeling is needed to provide best-estimate predictions of the potential consequences for potential consequences when the reactor vessel integrity is degraded or lost.
- Initiating event dependencies across systems is an important consideration for predicting end-states and modeling mechanistic source terms.
- The inventory tracking for multiple sources of radioactive material is not explicitly considered for existing hazard and safety analysis methods. The importance of a mechanistic source term code is heightened by this risk-informed insight.

Furthermore, MSTs and consequence analysis are discussed, along with their critical connection to the licensing process. The current capabilities for both MELCOR and the MELCOR Accident Consequence Code System (MACCS) are examined, and identified gaps are highlighted for MSRs in order to meet licensing needs. These gaps include the following:

Mechanistic Source Term Gaps:

- Molten salt equations-of state
- Circulating fuel point reactor kinetics
- Molten salt model for radionuclide transport

- Physics-based melt spreading
- Aerosol release characteristics, including generation rates, compositions, and sizes
- Volatile radionuclide release by vaporization and subsequent cooling leading to aerosol release
- Solubility of fission products for different salts as affected by contaminants such as water, oxygen in the air, and possibly concrete
- Thermodynamic and heat transfer properties

Consequence Assessment Gaps:

- Near-field atmospheric transport and dispersion modeling
- Reactor specific radionuclides and chemical forms
- Unique deposition behavior
- Decontamination methods and cost estimates

In order to start addressing these gaps, Argonne National Laboratories (ANL) has developed an experimental test plan to gather data for salt spill scenarios. A summary of this test plan is provided, along with a discussion on relevant data to be provided by these experiments. For MELCOR and MACCS to best inform MSR accident experiments, it is recommended that initial scoping studies be performed on the gaps identified in this report to best inform the relative importance of each item. Based on this assessment of relative importance, tailored experiments and simulations could be developed to specifically address the highest priority data gaps, ultimately leading to a refinement of analytical capabilities necessary to develop an MST and perform associated consequence assessments critical to licensing for MSRs.

2. OVERVIEW OF MOLTEN SALT REACTORS

Molten salt reactor systems can be divided into two basic categories: liquid-fueled Molten Salt Reactors (MSRs) in which the fuel is dissolved in the salt, and solid-fueled systems such as the Fluoride-salt-cooled High-temperature Reactor (FHR) where the fuel is solid and the coolant is molten salt. Both reactor types are included in this review and assessment.

2.1. Liquid-fueled Molten Salt Reactors

The liquid-fueled Molten Salt Reactor design is comprised of a reactor vessel with a liquid fuel and salt coolant mixture in the primary loop, and a coolant salt in both a secondary and potentially tertiary loop. Because the liquid fuel salt mixture is able to circulate through the primary loop to include the primary heat exchanger and primary system pumps, this creates a unique challenge for fission product inventory management. [1] Reactivity is controlled though top mounted control rods and negative reactivity coefficients for both the liquid fuel salt coolant mixture and graphite reflectors. Emergency systems to control reactivity include emergency dump tanks, which fill via gravity if an overheat condition causes a freeze plug of the salt mixture to melt.

Fission product buildup may be mitigated by an integrated chemical processing, or off-gas system, that removes fission products during operation to extend the necessary time intervals between refueling. It is estimated that the integrated chemical processing system allows the MSR design to obtain over 50% burnup of the nuclear fuel. [2] Risks identified for MSRs relevant to source term modeling and consequence analysis include tritium generation for systems containing lithium, and potential for corrosion of reactor mechanical components due to material incompatibility with the liquid fuel and salt coolant mixture. Figure 2-1 shows a pictorial description of a generic liquid-fueled MSR design from the Generation IV International Forum.

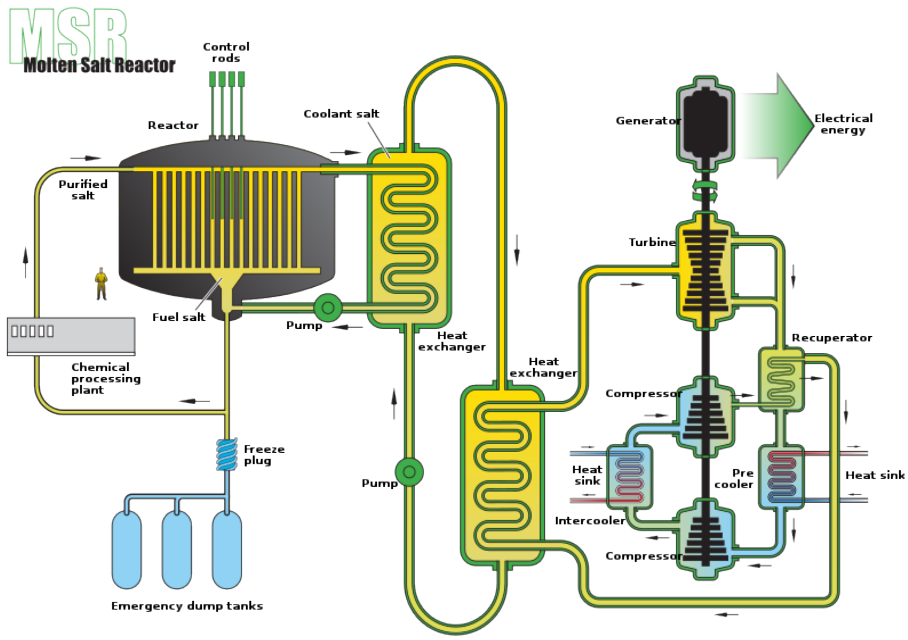

Figure 2-1: Diagram of a liquid-fueled Molten Salt Reactor developed as part of the Generation IV International Forum

2.2. Solid-fueled Molten Salt Reactors

The Fluoride-salt-cooled High-temperature Reactor (FHR) is an example of a solid-fueled, molten salt-cooled reactor. Figure 2-2 displays a schematic of the MK1 Pebble Bed FHR (PB-FHR). Like the latest Hight Temperature Gas Reactor (HTGR) concepts, the PB-FHR utilizes solid fuel tri-structural isotropic (TRISO) particles embedded in graphite pebbles. These pebbles are suspended in the flowing molten fluoride salt coolant in the primary system. [3] An advantage of this system is that actinides are retained within the TRISO particles, which have been shown to remain intact up to temperatures around 1600 C. [16] An additional consideration for FHR concepts, however, is the generation of tritium due to irradiation of fluoride salts. The magnitude of tritium estimated to be produced is generally larger than encountered for Light Water Reactors (LWRs), introducing a unique radiological hazard relative to LWR operating experience.

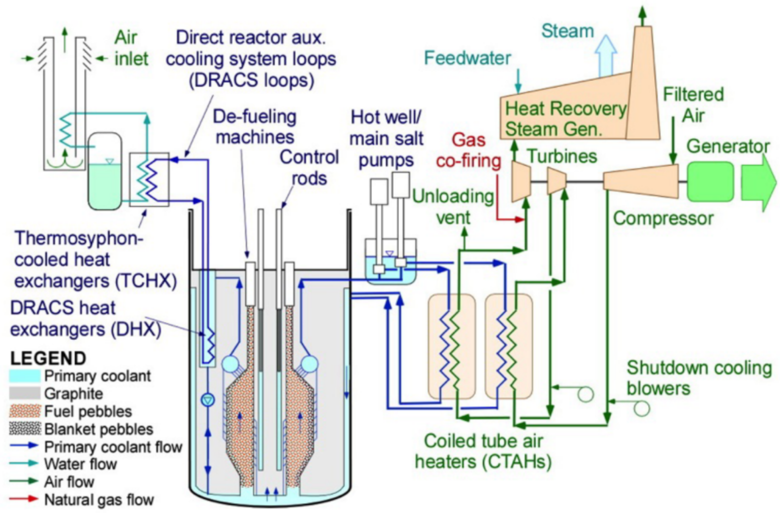

Figure 2-2: Mk1 PB-FHR Schematic [3]

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3. RISK ASSESSMENT AND LICENSING FOR MOLTEN SALT REACTORS

3.1. Background on Risk Assessment Activities

3.1.1. Industry and Regulatory Activities for Technology-Inclusive, Risk-Informed, Performance-Based Processes

The future design and development of Non-LWR technologies, including molten salt reactors, are expected to have increased levels of safety and higher safety margins. Demonstrating the safety and risk objectives can be achieved using a multitude of methodologies, tools, and capabilities. One such methodology is NEI 18-04, Revision 1, colloquially referred to as the Licensing Modernization Project (LMP). [4] The LMP provides guidance for a modern, technology-inclusive, risk-informed, and performance-based (TI-RIPB) process for selection of licensing basis events (LBEs); safety classification of structures, systems, and components (SSCs) and associated risk-informed special treatments; and determination of defense-in-depth (DID) adequacy for non-LWR technologies. Regulatory Guide 1.233 Revision 0 endorses NEI 18-04 Revision 1. RG 1.233 acknowledges that the LMP is just, "…one acceptable method for non-LWR designers to use when carrying out these [LMP process] activities and preparing their applications." [5]

Regardless of the methodology used by Non-LWR technology developers, there are some fundamental aspects of any risk assessment that are necessary, such as: identification of hazards; initiating events and scenarios challenging fundamental safety functions (i.e., reactivity control, heat removal, containment/confinement of radioactive material); safety analysis of SSCs; evaluation of defense-in-depth. Rarely, if ever, is just a single hazard or risk assessment method employed by a reactor designer. For example, although many nuclear power plants around the world use a probabilistic risk assessment (PRA), the PRA itself relies on results from HAZard and OPerability study (HAZOP), Failure Modes and Effects Analysis (FMEA), and deterministic analysis (i.e., modeling and simulation) to predict the consequences of the event sequences—also known as accident scenarios.

The relative lack of Non-LWR operating experience and SSC reliability data presents difficulties for using probabilistic risk assessments (PRA) in the design phases. Although

PRAs are well-suited to address uncertainties associated with a lack of data, for a large PRA model the analysts must be cautious when gathering insights and drawing conclusions from these models. While PRAs rely on probabilistic modeling, risk assessments need not necessarily be probabilistic in nature and can still provide risk-informed results and insights. However, similar to the lack of data issue with PRA, risk-informed results and insights must be carefully presented for any risk assessment, regardless of the quality and quantity of data.

3.1.2. Risk Assessment Attributes

Several attributes of PRA model development and analysis can also be leveraged for risk assessment, regardless of the data availability. First, the use of event trees and fault trees help organize complex arrangements of SSCs, human operator actions, and event sequences into digestible models. Systems analysis can be quite complex, especially when considering the interaction of humans, digital technology, physics, chemistry, and process components (i.e., pumps and valves). When considering the complex interactions between various SSCs during an event sequence, it can be difficult to keep track of all the known end states, thus, event trees help keep track of the possible end states for the analysts. Furthermore, end states can be grouped together depending on the analyst's metrics—typically they are grouped by frequency, such as in the LMP, but they may also be grouped by other metrics, such as consequence or qualitative system responses.

The second attribute common between PRA models and generic risk assessments are the risk-informed results and insights. Due to the inherent consequences associated with handling nuclear material, it's important to decompose the risks into results and insights that elucidate aspects of the design that are needed for maintaining the fundamental safety functions.

The third attribute of PRA models that can be leveraged for generic risk assessments is that PRA model development is structured and systematic. Utilizing structured and systematic processes helps reduce model uncertainty and ensure that the event sequences modeled in the risk assessment provide adequate scope for the analysis.

3.2. Generic MSR Risk Assessment

FOR PURPOSES OF DEMONSTRATING THE RISK ASSESSMENT METHODOLOGY, ONLY ONE MSR REACTOR TYPE, THE LIQUID-FUELED MSR, IS PRESENTED. THE ANALYSIS PERFORMED IS GENERIC AND FAR FROM EXHAUSTIVE. THE EMPHASIS OF THIS GENERIC ASSESSMENT IS TO HIGHLIGHT THE RISK-INFORMED INSIGHTS THAT CAN BE GAINED FROM LESS PROBABILISTIC MODELS. THE ANALYSIS IS BASED ON THE LIQUID-FUELED MSR DESIGN PRESENTED IN ACRONYMS AND DEFINITIONS

Abbreviation	Definition
ANL	Argonne National Laboratories
CVH	Control Volume Hydrodynamics
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4. INTRODUCTION

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Overview of Molten Salt Reactors. Most of the analysis that follows aligns with the LMP process but does not explicitly acknowledge the various steps.

4.1.1. Licensing Basis Event Selection

The first step in the risk assessment process is to select the LBEs. The initial list of initiating events should consider the applicability of NUREG/CR-3862 [6], NUREG/CR-5750 [7], and NUREG/CR-6928 [8] to the reactor concept. During the selection of licensing basis events, it's important to understand the potential failure modes of the reactor concept, how the plant would respond to such failure modes, and how protective strategies can be incorporated into formulating the safety design approach. In the design stages, this can be achieved using simple visual models such as safety function diagrams and functional event trees. Safety function diagrams are simple, hierarchical representations that illustrate which SSCs and passive features contribute to the fundamental safety functions. For the liquid-fueled MSR design concept, a safety function diagram is provided in **Error! Reference source not found.**. [1] Note that the safety function diagram is not representative of a system fault tree nor predicts DID features, such as redundancy/diversity of the design.

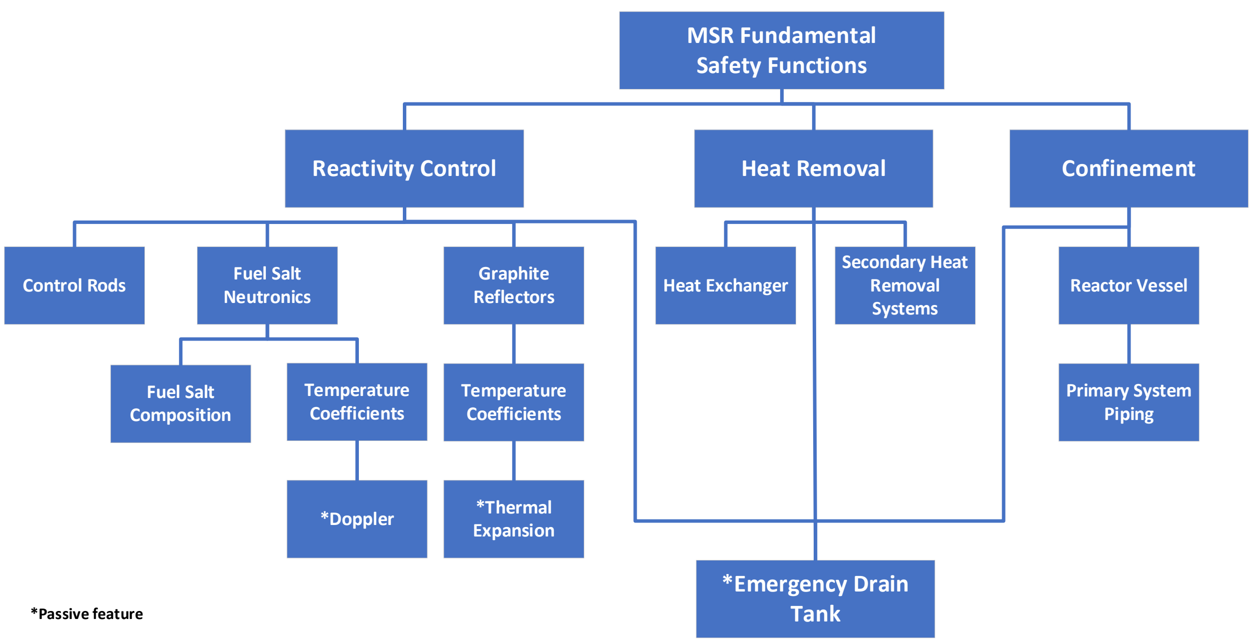

Figure 4-1. Liquid-fueled MSR safety function diagram [1]

Functional event trees illustrate the systems that are intended to respond during an event sequence to mitigate or arrest the event progression and consequences. Functional event trees are representative and as such, do not always characterize the chronological order of system response, although they could and should if the design stage has matured sufficiently. Similar to the safety function diagram, passive SSCs can be modeled, but the event sequence development and analysis for passive systems is complex and can be non-intuitive. Passive systems are typically omitted in the functional event tree if there is no potential deviation from their expected performance. For example, the Doppler feedback associated with fuel salt temperature is omitted as this phenomenon occurs regardless of the operating state and/or event sequence. Conversely, natural circulation can be dependent on system arrangement (i.e., specific valves opening/closing) and boundary conditions, which may or may not be conditional on preceding events.

The functional event tree illustrated in Figure 3-2 considers the primary systems listed in **Error! Reference source not found.**. Each branching creates a unique event sequence which results in an end state. The branching indicates whether the system succeeds in fulfilling its function (up branch) or fails to provide its function (down branch). No branching indicates that the system function is not needed during that event sequence. A few underlying assumptions in constructing the functional event tree in Figure 3-2 are described.

- Control rods are not modeled in the event tree. Operators are expected to insert the control rods, but the shutdown rods are the immediate events that are expected to respond during a transient or accident scenario.
- The “secondary heat removal system” in **Error! Reference source not found.** is considered a backup heat removal system. The details of this system are unknown at this time, but it is assumed that a backup heat removal system would be incorporated into the design.
- The reactor vessel encloses the entire reactor and primary system piping.
- The emergency drain tank is only used in specific event sequences, namely when the primary systems fail to respond. The emergency drain tank is represented by its own event tree.

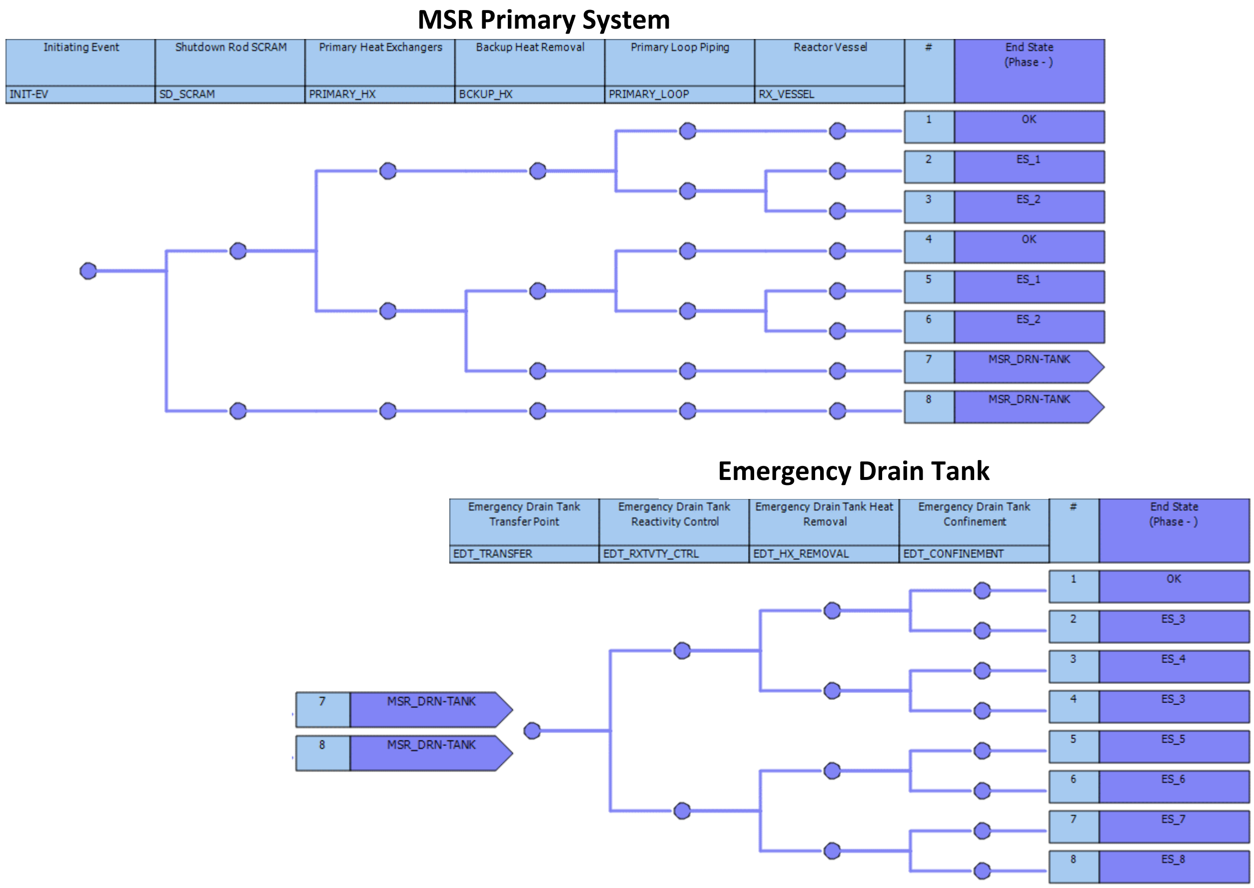

Figure 4-2. Liquid-fueled MSR functional event tree.

The End States (ES) on the right side of the functional event trees in Figure 4-2 are organized into event sequence families. At this level of the analysis, these event sequence families are simple, qualitative estimates of the potential consequences. The event sequence families are described below:

- OK. These event sequences are considered successful and have no or negligible radiological release.
- ES_1. These event sequences are categorized as sequences where reactivity control and heat removal are successful, but the reactor vessel integrity is degraded or lost.
    - Although there is no potential for radiological release from the primary system, there may be off-gas or chemical processing systems that could cause some radiological release.

- ES_2. These event sequences are categorized as sequences where reactivity control and heat removal are successful, but the primary system and reactor vessel integrity is degraded or lost.
- ES_3 through ES_8. These event sequences are a result of the emergency drain tank fundamental safety function responses. Each ES is treated separately, mainly due to the lack of design details for the emergency drain tank. Treating them separately at this stage is appropriate to avoid over-simplification of the consequences.

The top events in the functional event tree need to be expanded further to understand the events or chain of events that result in the loss of function for that specific top event. Further development of these events relies on additional hazard and safety analysis methodologies and processes. Hazard and safety analyses methods appropriate for this stage include HAZOP, FMEA, Process Hazard Analysis (PHA), and Master Logic Diagrams. The benefit of these approaches is that they are systematic, reproducible, and only as complete as the design itself. These studies are crucial for the risk assessment development as they provide the necessary basic event information, logic gate structure, events leading to loss of system function, and insights into how passive systems may respond during an event sequence.

4.1.2. Licensing Basis Event Evaluation

The end-states and resulting consequences for ES_1 and ES_2 are difficult to predict due to the importance of salt spills, aerosol and vapor generation in the reactor vessel, and transport of radionuclides outside of the primary system piping and reactor vessel. As the design matures and data becomes available, the frequency of these event sequences can be predicted probabilistically, but deterministic analysis will be needed to predict the consequences. Regardless of design maturity and data availability, these event sequences can be assessed using an integral systems analysis code such as MELCOR to characterize the mechanistic source term associated with these consequences.

> Risk-Informed Insight #1
>
> **Salt spill and splash modeling is needed to provide best-estimate predictions of the**

Note that in the functional event tree model in Figure 4-2, specific initiating events have not been assigned and the event tree logic is likely to change depending on the initiating event. For example, if a station-blackout (SBO) were to occur, it's likely that forced circulation associated with the primary heat exchangers would fail as a result of this initiating event. For this specific initiating event, the branching #'s 1, 2, and 3 in the MSR Primary System event tree would be collapsed. Thus, during an SBO, there is increased reliance on the Backup Heat Removal system. This lack of defense-in-depth further accentuates the importance of salt spill and splash modeling.

Risk-Informed Insight #2

Initiating event dependencies across systems is an important consideration for predicting

Consider another example where the initiating event is a break in the primary system piping. For this specific initiating event, branching #'s 1 and 4 in the MSR Primary System event tree would be collapsed. For this event tree, these are the only two OK end

Risk-Informed Insight #3

The inventory tracking for multiple sources of radioactive material is not explicitly considered for existing hazard and safety analysis methods. The importance of a

states, thus, there is some consequence associated with this event that must be considered. Also, during this initiating event, the event tree structure would change to go directly to the Emergency Drain Tank event tree. The response and procedures for this event sequence are unknown and the amount of liquid-fueled salt spilling into the reactor vessel would be dependent on the dynamic response. In other words, even though the emergency drain tank would be the final source of radioactive material, the consequences of this event sequence must consider the amount of radioactive material that spills into the reactor vessel. Event trees do not explicitly model multiple sources of radioactive material, but mechanistic source term codes such as MELCOR are developed for this specific purpose.

4.2. Risk-Informed Insights

The risk assessment developed and evaluated in this section is simple yet provides risk-informed insights into the design and mechanistic source term modeling needs. Given the emergence of the LMP approach, this places an increased reliance on mechanistic source term and consequence analysis modeling. Simple risk assessments can be performed to provide risk-informed insights into the design and informing scenario selection for future modeling.

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5. MECHANISTIC SOURCE TERM MODELING

Mechanistic source term modeling refers to prediction of radionuclide transport within and release from a nuclear system via a physics-informed, best-estimate plus uncertainty approach using an appropriate integral analysis tool.

The immediate concern is mechanistic regulatory source term modeling whereby the types and amounts of released radioactive material are calculated and utilized – supplemented by consequence assessment tools – for risk-informed regulatory decision-making in the context of radiological public health hazards. Mechanistic source term calculations for regulatory purposes are typically conducted for transient/accident scenarios falling within a design basis envelope that includes both normal operation and anticipated operational occurrences. This approach balances the risk profile, minimizes the overall risk, and lends credibility to the safety case of the nuclear system in question. Note that integral systems-level computational tools – facilitating large-scale uncertainty and sensitivity studies – can be used to:

- probe the space of credible design basis and beyond design basis scenarios,
- identify high-consequence and low-consequence phenomena and/or parameters,
- identify knowledge gaps and data needs,
- inform experimental programs in order to efficiently target gaps and data needs,
- help establish a technical basis for licensing assessments

MELCOR is a fully integrated, system-level computer code developed by Sandia National Laboratories (SNL) for the United States Nuclear Regulatory Commission (USNRC) with the primary objective of modeling the progression of severe accidents in both light water and non-light water nuclear power plants. Since the project began in 1982, MELCOR has undergone continuous development to address emerging issues, process new experimental information, and create a repository of knowledge for severe accident phenomena.

Despite its heritage supporting assessment and resolution of severe accident issues for LWRs, MELCOR has integrated, in a generalized manner, a broad range of models of phenomena to assess nuclear energy system behavior under normal and off-normal conditions. As a result, MELCOR is well suited to fill the role of an integral analysis tool for mechanistic regulatory source term calculations in MSR systems given that it:

- has new MSR-focused models/capabilities,
- has proven modeling capabilities for radionuclide and aerosol transport,
- is amenable to parametric studies (uncertainty, sensitivity),
- is fast-running, flexible, and adaptable, and
- is a tool familiar to the nuclear industry and its regulators.

MELCOR development for molten salt reactor modeling capabilities began in 2017. The development efforts have leveraged the extensive set of capabilities in MELCOR to represent the range of phenomena of relevance to normal and off-normal conditions in nuclear energy systems. Relatively focused modeling enhancements have been performed recognizing the extensive capabilities encapsulated within MELCOR. These include:

- a new equation of state for FLiBe working fluid,
- thermodynamic modeling improvements (e.g., ability to cope with salt freezing in control volumes),
- a circulating fuel point reactor kinetics model, and
- a new liquid-phase fission product transport model to characterize radionuclide chemistry, speciation, and transport modeling in and from salt pools

These development efforts have progressed sufficiently to enable demonstration of these capabilities through analysis of generic MSR systems (e.g., MSRE). Capability evolution will occur as necessary to resolve specific issues that emerge as MSR design and licensing progress. Supplementing development is a series of validation efforts currently underway for these new code capabilities.

5.1. MELCOR

A brief summary of each MSR-focused code enhancement is provided below, including include FLiBe equation-of-state (EOS) capabilities, circulating fuel point reactor kinetics, and the liquid-phase fission product chemistry and transport modeling that integrates with existing MELCOR radionuclide/aerosol transport modeling capabilities. Potential near-future model development activities are discussed as well.

5.1.1. FLiBe EOS

A working fluid equation of state library was created for LiF-BeF2 (FLiBe) using the soft sphere model. For molten salts, the Helmholtz equation is modified by an additional term to account for the fact that the original soft sphere model did not adequately model all degrees of freedom of stored energy for FLiBe. The property database is based on physical properties published by Oak Ridge National Laboratory (ORNL). Verification of the EOS library was again performed by a single volume test case that is heated internally at saturation conditions. The test shows (**Error! Reference source not found.** through Figure 4-6) that the equations are stable over a large range in pressure from 50 Pa up to 81 MPa where the critical pressure is 1.8 MPa.

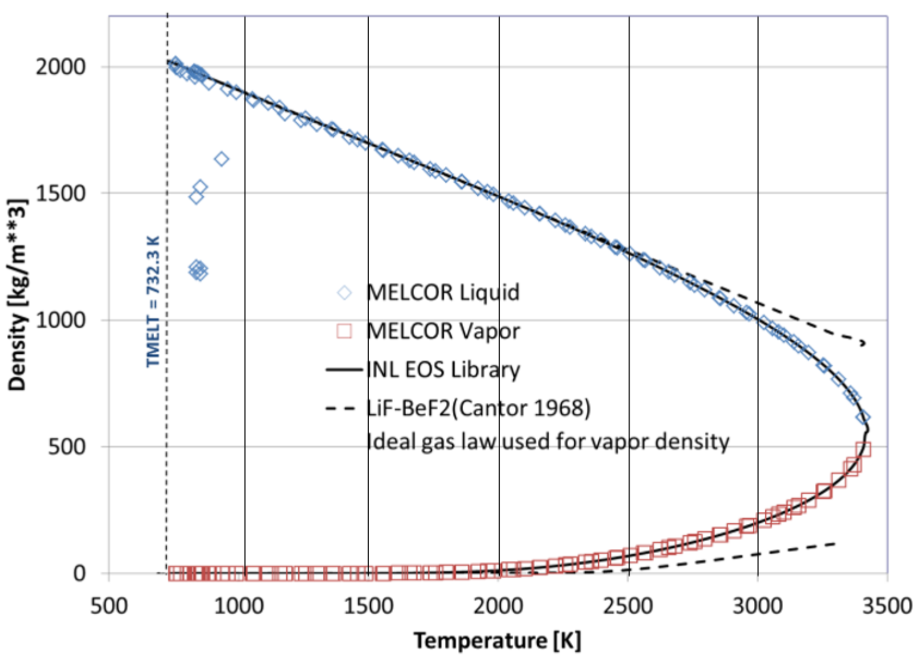

Figure 5-1: ***Li-BeF2 density curves at saturation***

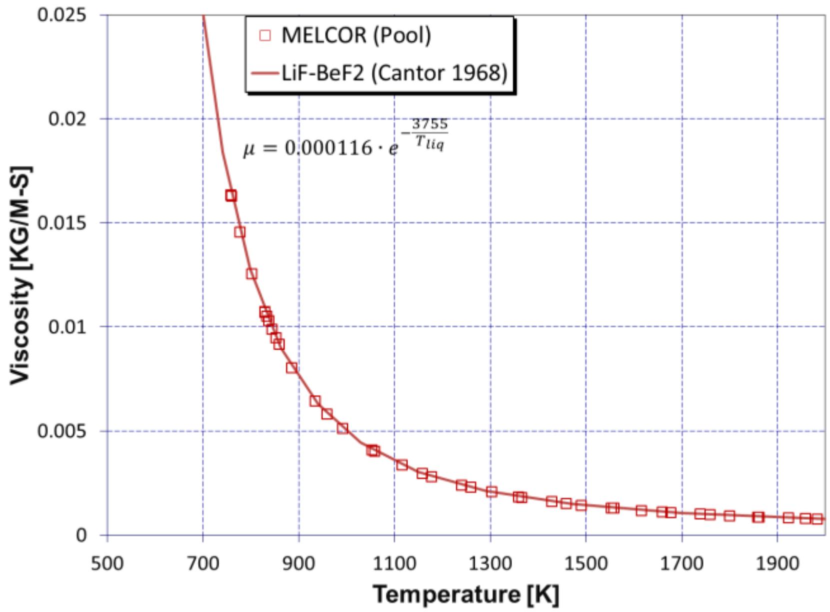

Figure 5-2. Viscosity curve for Lif-BeF2

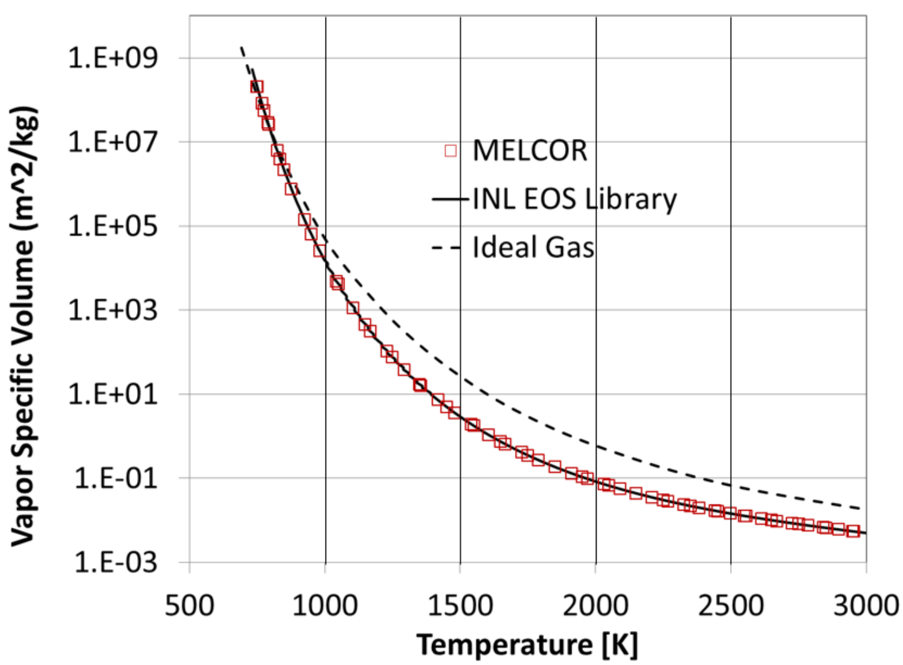

Figure 5-3. Vapor specific volume at saturation

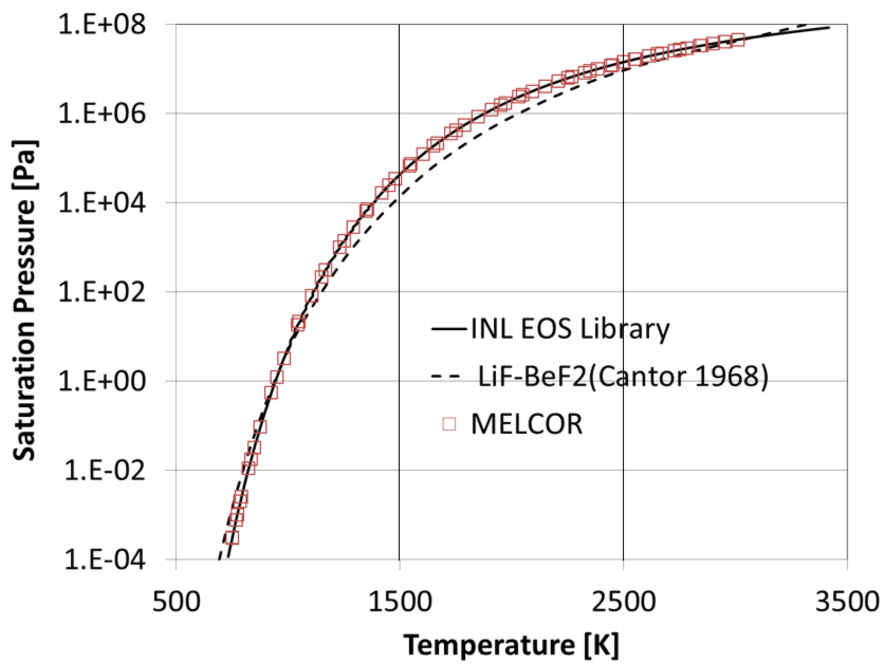

Figure 5-4. Saturation curve for LiF-BeF2

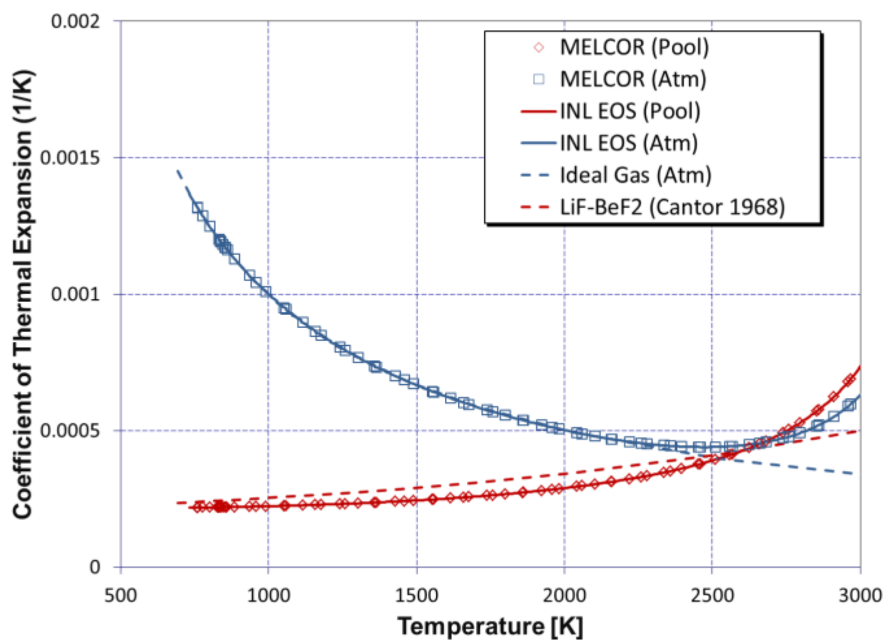

Figure 5-5. Coefficient of thermal expansion for LiF-BeF2

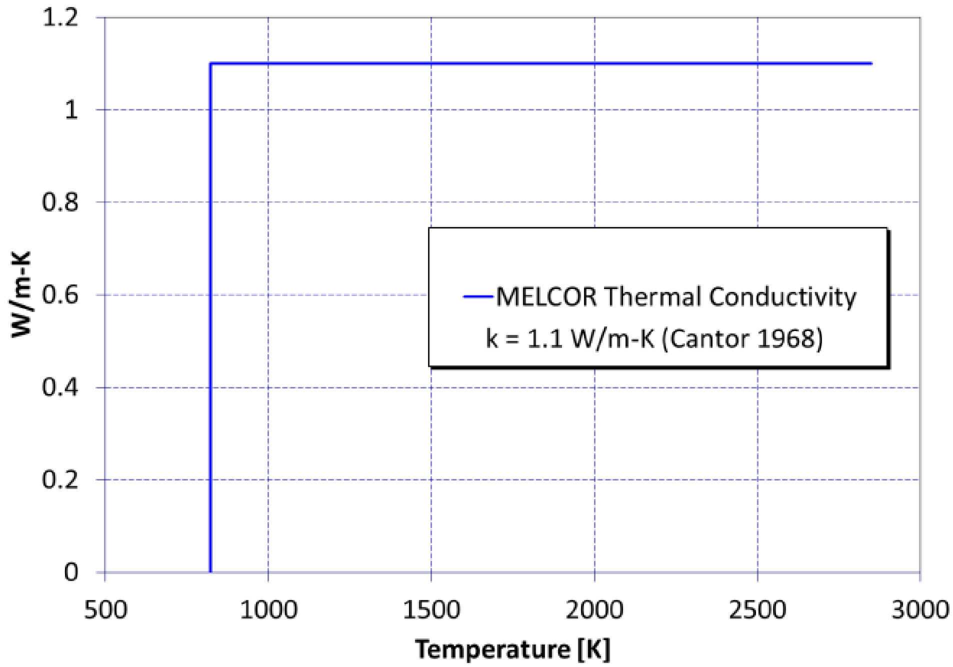

Figure 5-6. Thermal conductivity calculated for LiF-BeF2

5.1.2. Circulating Fuel Point Reactor Kinetics Equations

To improve MELCOR modeling capabilities for reactivity transients/accidents in an MSR system, a circulating fuel point kinetics model was implemented. A lumped approach to delayed neutron precursor accounting is consistent with a systems-level modeling philosophy. The delayed neutron precursor inventory is divided into an "in-core" cohort residing in the reactor core and an "ex-core" cohort residing in the reactor primary loop. There are six precursor groups per cohort.

The revised statement of conservation which applies group-wise for the delayed neutron precursors:

- In-core:
    - Precursors born by fission
    - Precursors lost by decay and by drift (advection out of the core, into the flow loop)

- Precursors gained by re-entry from the loop as characterized by a loop transit time

- Ex-core (loop):
    - Precursors gained by drift (advection out of the core, into the flow loop)
    - Precursors lost by decay during circulation (before re-entry to core)

There is still one equation for the fission thermal power magnitude P. There are now twelve equations for the two cohorts of delayed neutron precursors consisting of six groups each: six equations for C_i^C (core) and six equations for C_i^L (loop). The new set of PRKE's is:

$$\frac{dP(t)}{dt} = \left(\frac{\rho(t) - \overline{\beta}}{\Lambda}\right)P(t) + \sum_{i=1}^{6} \lambda_i C_i^C + S_0$$

$$\frac{dC_i^C(t)}{dt} = \left(\frac{\beta_i}{\Lambda}\right)P(t) - \left(\lambda_i + {}^{1}/_{\tau_C}\right)C_i^C(t) + \left(\frac{V_L}{\tau_L V_C}\right)C_i^L(t - \tau_L), \qquad for\ i = 1 \ldots 6$$

$$\frac{dC_i^L(t)}{dt} = \left(\frac{V_C}{\tau_C V_L}\right)C_i^C(t) - \left(\lambda_i + {}^{1}/_{\tau_L}\right)C_i^L(t), \qquad for\ i = 1 \ldots 6$$

$$\overline{\beta} = \beta - \left(\frac{\Lambda}{P(t)}\right)\sum_{i=1}^{6} \lambda_i C_i^L(t)$$

Where:

$P(t)$= Thermal power due to fission

C_i^C= delayed neutron precursor group i inventory/concentration in-core

C_i^L= delayed neutron precursor group i inventory/concentration ex-core (in loop)

S_0= Thermal power generation rate due to neutron source

$\rho(t) = \frac{k-1}{k}$= Reactivity for k the effective multiplication factor

$\overline{\beta}$= Effective delayed neutron fraction

β= Delayed neutron fraction (static, in absence of drift effects)

$\Lambda = {}^{1}/_{\nu V \Sigma_f}$= Neutron generation time

$\tau_{C/L} = {}^{M_{C/L}}/_{\dot{m}}$ = Residence time of precursors (core, loop, respectively)

$V_{C/L}$= Fluid volume (core, loop, respectively)

λ_i= Decay constant of delayed neutron precursor group i

Note that the gain of in-core precursors by in-loop precursor re-entry involves a time-shifted term, i.e. the gain of in-core precursors at time t depends on in-loop precursor concentration at $t - \tau_L$. Therefore, this term may be regarded as a constant source when solving the system of equations.

5.1.3. Liquid-Phase Fission Product Chemistry and Transport Model

Liquid-phase fission product chemistry and transport modeling is a recent addition to MELCOR radionuclide transport modeling capability meant to address the special concerns associated with non-LWR systems, such as MSRs and liquid metal fast reactors. Radionuclide mass is organized into chemical classes of elements as normal, but several new "forms" are introduced in the context of radionuclides in a liquid-phase medium (e.g., a salt pool):

- Soluble/dissolved form
- Colloid form
- Floating colloid form
- Colloid form deposited on heat structure
- Colloid form deposited on pebble surfaces (pebble bed salt-cooled reactor designs)

These new forms apply exclusively to radionuclide inventory residing in a salt pool and/or associated with structures (heat structure surfaces, pebble fuel element surfaces) submerged in a salt pool. Compatibility with existing RN1 package modeling methodology is preserved. Radionuclide class mass may transition between liquid pool forms; it may also transition between different liquid pool forms and conventional MELCOR radionuclide forms (e.g., aerosol and vapor radionuclides in a gaseous medium).

5.1.4. Physics-Based Melt Spreading

Attached to the MELCOR Cavity (CAV) physics package is a debris spreading model that considers a viscous and gravitational force balance. It ordinarily applies in the context of ex-vessel core debris modeling for light water reactors but could potentially be adapted for other purposes such as salt pool spreading after a spill.

Beginning with the equation for stokes flow in axisymmetric cylindrical geometry:

$$g\frac{\partial H}{\partial r} = \left(\frac{\mu}{\rho}\right)\frac{\partial^2 u_r}{\partial z^2}, \qquad for\ u_r = \frac{dr}{dt}, the\ spreading\ velocity$$

Where:

H= Pool cylinder height

$u_r = \frac{dr}{dt}$ = Pool spreading velocity

r = radial coordinate

z = axial coordinate

ρ = density

μ = viscosity

g = gravitational constant

Seeking a solution with dimensional analysis leads to the result for spreading radius:

$$R(t) = R(t_0) + \left[\left(\frac{2}{\pi}\right)^{3/8}\left(\frac{1}{8}\right)^{7/8}\right]\left(\left(\frac{1}{8}\right)\left(\frac{\rho g V^3}{\mu}\right)(t - t_0)\right)^{1/8}$$

Where:

$R(t)$= Pool radius

V = volume of pool cylinder

Clearly the salt pool properties (density, viscosity) must be known. The stand-alone spreading model in this form implies adiabatic spreading (no heat transfer between the pool and surroundings).

5.1.5. Brief Overview of Relevant MELCOR Code Packages

The Control Volume Hydrodynamics (CVH) package is a basic physical phenomena module. It models, in part, the thermal-hydraulic behavior of all hydrodynamic materials that are assigned to control volumes in a calculation. Control volume altitudes (relative to some chosen reference) as well as material volumes are specified by CVH input. The initial thermodynamic states of all control volumes are defined by CVH input as are any energy or material sources/sinks.

The Flow Path (FL) package is a basic physical phenomena module that works in tandem with the CVH package to predict thermal-hydraulic response. The FL input defines all characteristics of the control volume connections through which hydrodynamic material can relocate. The FL package is concerned with momentum and heat transport of single or two phase material as it moves from one control volume to another. Friction losses (e.g. to pipe walls), form losses, flow blockages, valves, and momentum sources (e.g. pumps) are defined through the FL package.

The Heat Structure (HS) package is another basic physical phenomena module that calculates heat conduction within any so-called heat structures. The structures are intact, solid, and comprised of some material with some definite geometry. The HS package also models energy transfer at a heat structure surface. This might include convection heat transfer to hydrodynamic material of an adjacent control volume or radiation heat transfer to separate heat structures.

The Decay Heat (DCH) package is a basic physical phenomena module. It is responsible for modeling the decay heat associated with any present radionuclide inventories in a calculation.

The Control Function (CF) package is a support functions module. It can be leveraged to create user-defined functions for use by the physics packages unique to an analysis. Real-valued control functions return a real value (i.e. floating point value), while logical control functions return one of two integer values that are interpreted as either "true" or "false". Most mathematical and logical functions available in modern Fortran are available for use in the CF package.

The Tabular Function (TF) package is a support functions module. Tabular functions are utilized when definition of some dependent variable (e.g., decay heat) is required as a tabular function of some independent variable (e.g., time from the initiating event or temperature).

The Cavity (CAV) package is traditionally used for ex-vessel modeling of oxidic and metallic core debris. It entails similar modeling capabilities (heat transfer, chemistry, spreading) to the CORQUENCH and MELTSPREAD codes. It has not yet been adapted for application beyond the space of ex-vessel debris modeling for LWR systems.

5.2. Data Needs for Mechanistic Source Term Modeling

An integral analysis tool like MELCOR can help to address issues surrounding data needs for mechanistic regulatory source term modeling. There are indeed a few questions one must consider when assembling lists of data needs and prioritizing them in view of limited experimental and/or computational resources. In the context of mechanistic regulatory source term modeling with integral systems-level analysis tools for licensing purposes, these questions include:

- What transient/accident scenarios are credible and relevant to evaluating the overall risk profile of the nuclear system?
- For each plausible/credible scenario identified:
    - What physical phenomena are relevant to assessing accident progression and evaluating radiological source terms?
    - Do any modeling gaps exist in representing relevant physical phenomena?
    - To what extent are any phenomenological modeling capabilities validated?
    - If models/capabilities exist for relevant physical phenomena and are validated, do gaps exist with respect to adequately informing/specifying them for the application?

- If models/capabilities are available and validated, and data is available to inform/specify them, do prevailing uncertainties in analyses impact regulatory decisions?

Computations are generally far less expensive than experiments, so computations ought to be leveraged to first identify knowledge gaps and data needs. Insights gained from this evaluation process, can be used to determine the relative importance of gaps/data needs as well as any necessity to reduce the level of uncertainty. The data needs screened by computations as relatively higher consequence/uncertainty then become the logical targets of a more expensive experimental program intended to reduce uncertainty and/or address the specific need.

Lists of MSR-related data needs (encompassing the entirety of MELCOR MSR models/capabilities) will be presented for two categories of MSR accident/transient scenarios:

1) the salt spill scenario dictating the three proposed ANL salt spill experiments, and
2) other plausible MSR scenarios

The “other” category assumes scenarios besides salt spills could reasonably have a place in the critical path to a near-term licensing basis for MSRs pending further investigation.

A survey of pertinent MELCOR MSR-related models/capabilities is given along with anticipated data needs. The data needs are mostly code and/or user inputs.

5.2.1. Salt Spill Scenario: MELCOR Models/Capabilities and Data Needs

In view of the ANL salt spill experimental plan and in anticipation of upcoming MELCOR scoping calculations, a list of relevant MELCOR models and capabilities was compiled along with corresponding data needs. The list is organized by MELCOR model/capability according to code physics package. Data needs are itemized for each identified model/capability.

5.2.1.1. CVH/FL Models/Capabilities and Data Needs

Pertaining to the CVH and FL code packages:

- Molten salt EOS model to include salt freezing
    - Validation data and basic scientific research
- Ordinary thermodynamic and flow (phasic velocity equation) model
    - Thermodynamic state inputs
    - Flow path inputs
- Advection of form-wise radionuclide class mass
- Pool/atmosphere energy exchange (mutually, with surroundings)
    - Heat transfer coefficient information
    - Radiation heat transfer information
- Salt pool radionuclide release to atmosphere
    - Characterization of solubilities
    - Characterization of aerosol generation modes (splash, slosh, bubble burst)
- If representing fission product chemistry and transport in a liquid-phase medium, specification of transport rates between radionuclide forms in the liquid-phase medium
    - Characterization of transitions between soluble/dissolved and insoluble colloid
    - Characterization of colloid surface deposition
- Aerosol sourcing capabilities (soluble form in pool to aerosol form in atmosphere)
    - Aerosol generation rates off pool from various modes/mechanisms
    - Size distributions
- Characterization of salt blockage formation in pipes

5.2.1.2. HS Models/Capabilities and Data Needs

Pertaining to the HS package:

- Horizontal surface heat transfer to pool above
    - Nusselt number and/or heat transfer coefficient data (liquid pool, freezing pool)
- Vertical/inclined surface resuspension
    - Characterization of lift-off capability
    - Size redistributions of deposited radionuclide inventory

- Decay heat due to deposited radionuclides
    - Characterization of deposition trends (phoretic effects)
- Salt pool and structural substrate interactions and/or off-gassing
    - Chemical interactions
    - Heat transfer/Nusselt number correlations

5.2.1.3. DCH/RN1 Models/Capabilities and Data Needs

Pertaining to the DCH/RN1 package:

- Molten Salt Model (MSM)
    - Form-wise behavior in salt pool
    - Chemistry/speciation
- Decay heat (specific decay power by class)
    - Initial radionuclide class masses
    - Time histories of specific decay power by radionuclide class
- Fission product chemistry in atmosphere
    - Characterization of especially consequential chemical interactions for source term
- Conventional RN1/MAEROS
    - Characterization of agglomeration, condensation/evaporation, aerosol geometry and shape factors, appropriate size binning
    - Deposition kernel characterization

5.2.1.4. CAV Models/Capabilities and Data Needs

Pertaining to the CAV package and assuming future CAV development to permit application in the context of molten salt rather than oxidic/metallic core debris:

- CAV/CORCON has a litany of sub-models that would benefit from experimental investigations (along the same lines as MELTSPREAD)
    - Heat transfer
    - Chemistry
    - Steel and concrete interactions

    - Radionuclide release and aerosol generation
- Physics-based spreading model
    - Thermophysical/transport properties of salt
    - Validation data appropriate for adiabatic salt spill spreading

5.2.2. Other Scenarios: MELCOR Models/Capabilities and Data Needs

MELCOR would be a fitting analysis tool for other transient/accidents scenarios within the critical path to a near-term MSR licensing basis besides salt spills. Therefore, a list of potentially relevant MELCOR models and capabilities was compiled along with anticipated data needs for these "other than salt spill" scenarios. Only the non-overlapping models/capabilities with respect to salt spills are mentioned below, but most or all the identified models/capabilities/needs for salt spills may apply to other scenarios.

5.2.2.1. CVH/FL Models/Capabilities and Data Needs

Pertaining to the CVH and FL code packages:

- Fluid fuel point reactor kinetics equations
    - Kinetics parameters
        - Neutron generation time
        - Delayed neutron precursor grouping parameters
    - Feedback models
        - Empirical model for Doppler feedback given neutron spectrum
        - Miscellaneous feedback effects other than Doppler (temperature) and flow
    - Validation data

6. CONSEQUENCE ANALYSIS MODELING

6.1. MACCS Accident Consequence Code System (MACCS)

The MELCOR Accident Consequence Code System (MACCS) was developed for the United States Nuclear Regulatory Commission (NRC) by SNL to calculate health and economic consequences following a release of radioactive material into the atmosphere. MACCS accomplishes this by modeling the atmospheric dispersion, deposition, and consequences of the release, which depend on several factors. These include the source term, weather, population, economic, and land-use characteristics of the impacted geographical area. From these inputs, MACCS determines the characteristics of the plume, as well as ground and air concentrations as a function of time and tracked radionuclide.

Users may select an atmospheric transport model based on a simpler straight-line Gaussian plume segment model or a more detailed hybrid Lagrangian/Eulerian method. This latter model is an enhancement added in June 2020 that couples MACCS with Hybrid Single-Particle Lagrangian Integrated Trajectory (HYSPLIT), an atmospheric transport and dispersion modeling system developed by the National Oceanic and Atmospheric Administration (NOAA). Along with atmospheric dispersion, MACCS also calculates the health effects of exposure, impacts on the food chain, and the economic impact following an accident. More specifically, the MACCS code suite models the following:

- Atmospheric transport and dispersion
- Wet and dry deposition
- Probabilistic treatment of meteorology
- Exposure pathways
- Emergency phase, intermediate phase, and long-term phase protective actions
- Dosimetry
- Health effects
- Economic impacts

MACCS has been routinely updated and modernized by both SNL and the U.S. NRC for over 40 years. The user base includes both domestic and international users, including the NRC, DOE and their contractors, several research organizations, nuclear industry licensees/applicants, and academic institutions. Primary uses of MACCS include performing regulatory cost-benefit analysis of Severe Accident Mitigation Alternatives (SAMAs) and Severe Accident Mitigation Design Alternatives (SAMDAs), evaluation of emergency planning, Level 3 PRA studies, consequence studies, documented safety analyses, and other risk-informed activities. Also, of significance, MACCS is one of few existing tools capable of treating, within a probabilistic framework, all of the technical elements of the ASME/ANS RA-S-1.3-2017 Standard for Radiological Accident Offsite Consequence Analysis (Level 3 PRA) to Support Nuclear Installation Applications. As such, MACCS naturally fills the role of a consequence evaluation tool for the non-LWR PRA standard as well.

6.2. Data Needs for Molten Salt Reactors

A key component of consequence analysis modeling is accurately characterizing the source term outside the site boundary, which defines the magnitude and timing of what is released into the atmosphere. Therefore, a full characterization of the radionuclides released, their chemical forms, particle size distributions, and energy of release in essential. Furthermore, once released into the atmosphere, a thorough understanding of transport and deposition behavior is essential. For MSRs, deposition and transport behavior, to include potential absorption and re-vaporization for tritium is a current knowledge gap in need of resolution in order to accurately characterize consequences of MSR releases. Finally, when it comes to determining long term consequences, potential differences in decontamination methods need to be considered along with changes to released radionuclides and chemical forms. These identified gaps in consequence assessment modeling are consistent with the "NRC Non-Light Water Reactor (Non-LWR) Vision and Strategy, Volume 3 Computer Code Development Plans for Severe Accident Progression, Source Term, and Consequence Analysis." [9]

6.2.1. *Released Radionuclides and Associated Chemical Forms*

Currently, 71 radionuclides are typically used for LWR consequence analysis modeling in MACCS, in accordance with the NRC's State of the Art Reactor Consequence Analyses (SOARCA) Project. [10] However, the flexibility of MACCS allows for a much greater selection of 150 radionuclides, which can be selected from a list of 825 radionuclides. A study was conducted in 2020-2021 which analyzed which additional radionuclides would potentially require inclusion in advanced reactor consequence analysis modeling, which included an analysis on MSRs. [11] This study took into account estimates for reactor inventories and activation products, which is an area in need of further refinement outside of MACCS. This study also examined a range of fuel types, including liquid-fueled, solid-fueled, Th-232, U-233, and Pu-239. Without a determined inventory, this study utilized data from MSRE [12] to provide a list of radionuclides and associated chemical forms with the potential to be released to the atmosphere to be modeled for MSRs, in addition to what is currently modeled for LWRs.

Criteria used in determining this list included the half-life and quantity of release. Half-life being sufficiently long to not decay prior to reaching the site boundary, and sufficiently short to pose a potential health risk. Similarly, with quantity of release, radionuclides were chosen with sufficient quantities to pose a potential health risk. The results of this study are displayed in Tables 5-1, 5-2, and 5-3, which highlight several additional radionuclides to be included for atmospheric transport and dispersion modeling for MSRs depending on fuel and salt type. Follow-on efforts are planned in order to prioritize this list further based on potential for release into the atmosphere, and potential to cause health consequences.

Table 6-1: Recommended additional nuclides for inclusion in off-site consequence analysis for fluoride salt MSRs, showing corresponding chemical group in MACCS [11]

Nuclide	Corresponding Chemical Group	Nuclide	Corresponding Chemical Group
H-3	Proposed New Group	Sb-128	Cadmium Group
Na-22	Alkali Metal	Te-125m	Chalcogens
Na-24	Alkali Metal	Te-133m	Chalcogens
As-77	Cadmium Group	Te-134	Chalcogens
Se-81	Chalcogens	Xe-131m	Noble Gas

Nuclide	Corresponding Chemical Group	Nuclide	Corresponding Chemical Group
Se-81m	Chalcogens	Xe-133m	Noble Gas
Se-83	Chalcogens	Pr-146	Trivalents
Br-83	Halogen	Pm-147	Trivalents
Br-84	Halogen	Pm-148m	Trivalents
Kr-83m	Noble Gas	Pm-149	Trivalents
Nb-93m	Trivalents	Pm-151	Trivalents
Pd-109	Platinoids	Sm-151	Trivalents
Pd-112	Platinoids	Sm-153	Trivalents
Ag-111	Tin Group	Eu-154	Trivalents
Cd-113m	Cadmium Group	Eu-155	Trivalents
Cd-115m	Cadmium Group	Eu-156	Trivalents
Sn-117m	Tin Group	Eu-157	Trivalents
Sn-119m	Tin Group	Ra-224	Noble Gas
Sn-121m	Tin Group	Th-228	Tetravalents
Sn-123	Tin Group	U-232	Uranium Group
Sb-125	Cadmium Group	Pa-233	Tetravalents
Sb-126	Cadmium Group		

Table 6-2: Recommended additional nuclides for inclusion in off-site consequence analysis for chloride salt MSRs, showing corresponding chemical group in MACCS [11]

Nuclide	Corresponding Chemical Group	Nuclide	Corresponding Chemical Group
H-3	New Proposed Group	Te-125m	Chalcogens
As-77	Cadmium Group	Te-133m	Chalcogens
Se-81	Chalcogens	Te-134	Chalcogens
Se-81m	Chalcogens	Xe-131m	Noble Gas
Se-83	Chalcogens	Xe-133m	Noble Gas
Br-83	Halogen	Pr-146	Trivalents
Br-84	Halogen	Pm-147	Trivalents
Kr-83m	Noble Gas	Pm-148m	Trivalents
Nb-93m	Trivalents	Pm-149	Trivalents

Nuclide	Corresponding Chemical Group	Nuclide	Corresponding Chemical Group
Pd-109	Platinoids	Pm-151	Trivalents
Pd-112	Platinoids	Sm-151	Trivalents
Ag-111	Tin Group	Sm-153	Trivalents
Cd-113m	Cadmium Group	Eu-154	Trivalents
Cd-115m	Cadmium Group	Eu-155	Trivalents
Sn-117m	Tin Group	Eu-156	Trivalents
Sn-119m	Tin Group	Eu-157	Trivalents
Sn-121m	Tin Group	U-237	Uranium Group
Sn-123	Tin Group	Pa-233	Tetravalents
Sb-125	Cadmium Group	Pu-242	Tetravalents
Sb-126	Cadmium Group	Cm-243	Trivalents
Sb-128	Cadmium Group	Cm-245	Trivalents
		Cm-246	Trivalents
		Am-242m	Trivalents
		Am-243	Trivalents

Table 6-3: Recommended additional nuclides for inclusion in off-site consequence analysis for solid-fueled MSRs, showing corresponding chemical group in MACCS [11]

Nuclide	Corresponding Chemical Group
H-3	Proposed New Group
C-14	Proposed New Group
Ag-110m	Tin Group
Sb-125	Cadmium Group
Pm-147	Trivalents
Sm-151	Trivalents
Eu-154	Trivalents

Nuclide	Corresponding Chemical Group
Eu-155	Trivalents
Pu-242	Tetravalents
Cm-244	Trivalents
Cm-245	Trivalents

6.2.2. Chemical Forms and Unique Deposition Behavior

This same study also examined in what chemical forms these radionuclides may be released, which again also depends on the reactor inventory and fuel composition, and on the chemistry within the reactor. Once more refined MSR inventory data are available, additional refinement in this area is necessary to accurately characterize atmospheric transport and dispersion as some chemical forms are reactive and/or hygroscopic, and therefore may evolve after release and alter the deposition behavior. Currently, the deposition velocity in MACCS is constant for a particular chemical group and particle size bin, which takes into account surface roughness and windspeed. However, this treatment does not take into account evolving species with the potential to change chemical forms, and therefore change deposition velocities. Furthermore, this method also does not take into account varying shape factors, and simply models all particles with a shape factor of unity representing a perfect sphere. An alternative, resistance model to represent deposition velocities has been proposed to account for these characteristics.

Changes in radionuclides, chemical forms, and their associated particle sizes and deposition behavior are all important for not only characterizing concentrations, but also for accurately characterizing health effects following exposure. Different chemical forms can lead to solubility changes in the human body. Furthermore, dose conversion factors are based on a 1-micron median particle diameter, which may require re-evaluation for a different range of particle sizes along with chemical forms, all of which have the potential to impact dosimetry and health effect calculations.

Furthermore, the addition of new radioactive chemical groups and non-radioactive chemical hazards would need to be considered. Tritium in particular is expected to be present in MSR systems due to neutron absorption of lithium, however the transport behavior of tritium is not currently modeled in MACCS. A new chemical class would be required to characterize the atmospheric dispersion of tritium, taking into account the absorption and re-vaporization of tritiated water vapor on surfaces, along with associated dose conversion factors to model the resulting health effects. For non-radioactive chemical hazards, an analysis of potential chemical hazards arising from MSR source terms would also need to be considered, which may include the release of beryllium and chlorine gas. Non-radioactive chemical hazards are not currently treated within MACCS, but have been treated by CHEM-MACCS in the past, which could be re-instituted if deemed necessary for modeling the release of MSR source terms. [9]

6.2.3. Off-Site Decontamination Methods

The economics of decontamination are driven by the cost effectiveness of decontamination methods compared to the interdiction or permanent condemnation of the property. Decontamination methods are well characterized for LWRs, both in terms of effective methods to decontaminate and their associated costs. However, if the radionuclides and associated chemical forms are different, as anticipated, different decontamination methods will need to be developed along with estimates of their cost to accurately factor into economic consequence modeling. Tritium is good example here as well. Tritium permeates easily through metals, creating a challenge for decontamination methods. Furthermore, decontamination estimates for MACCS are currently based on rural and suburban environments. With the potential that non-LWRs may be closer to urban environments, more complex structures and materials may need to be considered in refining decontamination models. [9]

6.2.4. Near-Field Modeling

Near-field modeling refers to atmospheric transport and dispersion modeling within 500 meters of the source. Within 500 meters of the source, dispersion phenomena including building wake effects and potential for recirculation cavity zones can cause higher concentrations. [9] Currently in MACCS, a simple model is used for building wake effects which scales the dispersion parameters based on the building dimensions, which can lead to conservative assessments for concentrations in the near-field. With the expectation that advanced reactors will have smaller source terms compared to their LWR counterparts, higher fidelity atmospheric transport and dispersion models focused closer to the source is of particular importance. Such analysis can be influential in determining appropriate Emergency Planning Zones (EPZs) for advanced reactors, which may be more appropriately set at a distance below the 10 mile EPZ used for LWRs.

To work towards closing this gap, the MACCS team is releasing MACCS v4.1 in July 2021 where the primary model enhancements are added options to better model near-field atmospheric dispersion. These near-field MACCS model improvements were motivated by a study conducted by SNL in 2019 that compared MACCS v3.11.6 to several near-field atmospheric transport and dispersion codes including QUIC, ARCON96, and AERMOD2. This study concluded that MACCS performed comparably for near-field atmospheric transport and dispersion modeling, and provided a conservatively bounding assessment compared to QUIC, ARCON96 and AERMOD. [13] These added options include the ability to:

- Model plume meander using the Ramsdell and Fosmire model
- Model trapping and downwash using the Briggs model, with options for specifying building parameters or buoyancy flux

Implementing these options reduces the conservatism in concentration calculations in the near field. However, these near-field modeling improvements currently only apply to the Gaussian Plume Segment model within MACCS. MACCS also integrates with HYSPLIT for a higher-fidelity Lagrangian particle tracking model, which requires further refinement of the minimum time step in order to be utilized for higher fidelity near-field modeling.

7. MOLTEN SALT SPILL EXPERIMENTS

7.1. Test Plan from Argonne National Laboratories

A postulated accident scenario for MSRs entails a rupture of the primary system causing a spill of the molten salt onto the floor of the containment. In order to better characterize such an accident scenario, Argonne National Laboratories (ANL) has developed a test plan focused on gathering information to better define the behavior of the bulk salt, salt-substrate interactions, and associated aerosols during this event on a very much smaller scale than anticipated for an actual MSR. In general, the setup for the experiment is depicted in Figure 6-1 below:

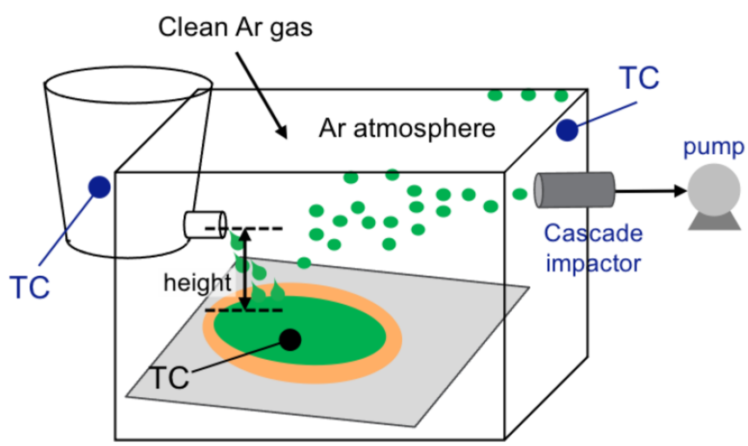

Figure 7-1: Argonne National Lab Salt Spill Experimental Setup [14]

The experimental setup includes an elevated and heated crucible of FLiNaK, which is then poured onto a tilted stainless steel substrate or stainless steel tube leading to a catch pan for substrate interactions. The whole apparatus in contained within an Argonne glovebox. Instrumentation includes wireless infrared cameras and visible cameras, multi-junction thermocouples, and a cascade impactor. Furthermore, SEM/EDS is planned for studying the composition after freezing has occurred. It is the goal that these experiments will capture data on: [14]

- Flow rate of pour.
- Temperature of salt in crucible during pouring.

- Leading-edge position over time.
- Covered area over time.
- Temperature of underside of steel substrate in and near flow path.
- Temperature salt surface (IR camera).
- Temperature of upper steel substrate surface out of flow path.
- Composition of frozen salt.
- Samples of condensed vapor that may collect on the distance marking rods (mass and compositions).
- Temperature, total pressure, and O_2/H_2O content of the glovebox atmosphere before and during test.
- Flow rate of salt through tubing.
- Temperature of catch pan and tubing.
- Temperature of salt in crucible, catch pan, and tubing.
- Time and location at which the tubing plugs with frozen salt.
- Extent of deformation of catch pan and tubing.
- Composition of cross section of frozen salt inside tubing.
- Compositional changes of collected salt that flows through tubing.
- Splash pattern that forms on substrate.
- Temperature of salt in the crucible and on the stainless steel substrate.
- Temperature of spilled salt surface over time.
- Temperature, total pressure, and O_2/H_2O content in spill containment box.

- Size distribution and abundance of aerosol particles collected by cascade impactor.
- Composition of aerosol particles.

7.2. Data needs of Importance for Mechanistic Source Term and Consequence Analysis Modeling

There are two types of radionuclide releases of concern for severe accidents, and those are vapor and aerosol. Non-condensable fission product gases such as Xe and Kr can be expected to be released in an accident. Aerosol containing radionuclides can be formed either directly from molten salt, or from volatile radionuclides released as vapor that later condense into an aerosol. It is the aerosol form that has much uncertainty and therefore in need of experimental data.

We envision a spill in which the salt is significantly above the reactor normal operating temperature. Spills can create much molten salt surface area exposed to an atmosphere. Compounds containing the fission products of cesium and iodine are the most likely volatile radionuclides, and therefore most likely to be released as a vapor. However, upon cooling these vapors can be expected to form aerosol particles. A schematic of this process is given below followed by a table listing the data needed to estimate this release mechanism and the status of the data.

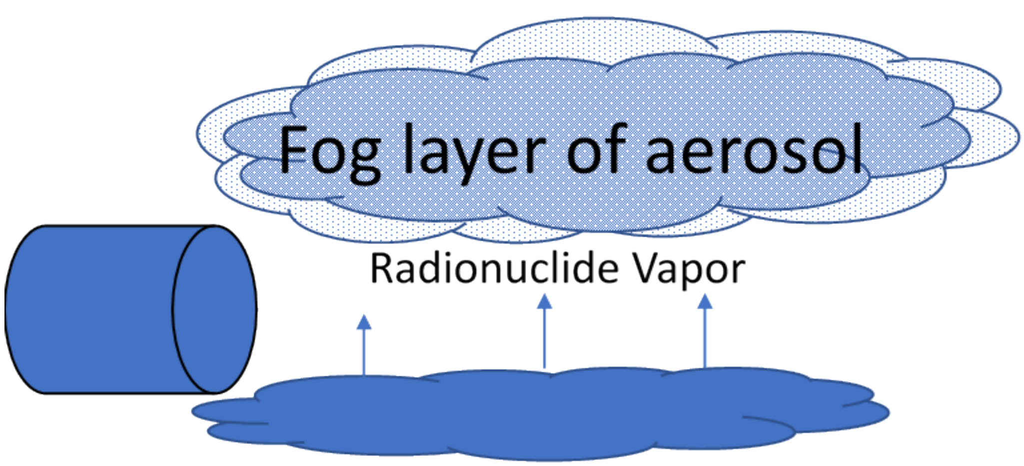

Figure 7-2: Radionuclide vapors and aerosols

Table 7-1: Data needs for volatile radionuclides

Data Needs	Status
Spill geometry, volume, salt temperature, and salt composition	Vendor-dependent but some nominal values needed
Substrate properties: thickness and extent, temperature, thermal conductivity, heat capacity, and density	Vendor-dependent but some nominal values needed
Salt physical properties (thermal conductivity, heat capacity, density, viscosity and surface tension)	Available for pure salts at operating temperatures. Need to verify extrapolations to higher temperatures. Contaminant effects due to air and water vapor exposure are unavailable and may be estimated.
Vapor pressure with temperature and salt composition, and vapor diffusivity in atmosphere	Estimated from thermodynamic database if available.

The second mechanism for aerosol release is the entrainment of gas that forms surface bubbles that rupture. Gas may be entrained by the spill, or by agitation of the molten salt upon impacting the substrate. When the bubbles burst, for aqueous solutions the particles formed from the thin film of the bubble can be respirable. [15] Since the salt solution contains radionuclides, the particles formed from the solution will therefore contain radionuclides. We found no data on the behavior of bubbles in molten salt. Furthermore, we found no data on the bubble formation rate for different levels of molten salt agitation. Data are needed for this phenomenon to either discount this process for molten salts, or to quantify the amount of direct aerosol release.

7.3. Recommendation Gap Closure

For MELCOR and MACCS to best inform MSR accident experiments, it is recommended that initial scoping studies be performed on the gaps identified in this report to best inform the relative importance of each item, with priority assigned based on relevance to licensing applications. Based on the assessment of relative importance and relevance to licensing, tailored experiments and simulations could be developed to specifically address the highest priority data gaps. This concept is displayed in Figure 6-3 below:

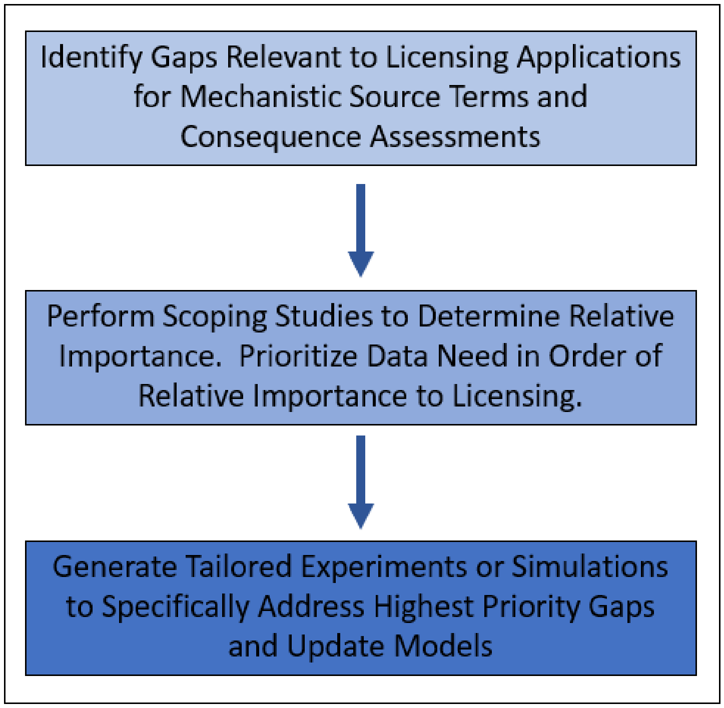

Figure 7-3: Recommended Pathway for Gap Closure

8. SUMMARY

This report highlights the gaps in mechanistic source term and consequence assessment modeling for MSRs. The current capabilities for MELCOR and the MELCOR Accident Code System are discussed, along with updates needed to address specific needs for MSRs. Although a test plan developed by Argonne National Laboratories attempts to address some of these gaps, most will require additional attention. For MELCOR and MACCS to best inform MSR accident experiments, it is recommended that initial modeling scoping studies be performed to prioritize these gaps, which would lead to more focused experimental or simulation closure plans. This report satisfies the DOE NE Milestone M2RD-21SN0601061 to leverage MELCOR and MACCS to identify parameters of importance for source term assessments for salt spill experiments.

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