TERRESTRIAL
ENERGY USA

Modeling and Simulation Activities Related to Source Term for IMSR Design Basis Accidents

Whitepaper

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Abstract

TEUSA's licensing objective is to obtain a Standard Design Approval (SDA) for the IMSR Core-unit. A necessary component of a 10 CFR Part 52 SDA application for the IMSR Core-unit is the identification and description of the radiological source terms that will be used to demonstrate that, in the event of a postulated design basis accident, the regulatory criteria for radiological exposure to the general population will not be exceeded. This white paper summarizes the methodology, key analysis parameters, and generic model of a MSR facility that are important for the generation of a radiological source term that is to be used in calculating the radiological consequences following a postulated design basis accident. The evaluation of radiological consequences following postulated design basis accidents is a necessary element of an application for a license. Any application for a license must demonstrate that the regulatory limits for exposures to the general population of radionuclides released following postulated design basis accidents will not be exceeded. This white paper discusses the key phenomenological attributes of molten fuel salt that contribute to the potential release of volatile radionuclides. This document also discusses key uncertainties that must be considered in estimating a mechanistically derived radionuclide source term. The application of the methodology and simulations specific for the IMSR400 will be described in a future topical report.

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Non-Proprietary

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Abbreviations & Acronyms

ANL – Argonne National Laboratory

AOO – Anticipated Operational Occurrence

BOL – Beginning of Life

B4C – Boron Carbide

CAPPHAD – CALculationof PHAsed Diagramd

CHT – Convective Heat Transfer

CFR – Code of Federal Regulations

Cs - Cesium

CsI – Cesium Iodine

DBA -- Design Basis Accident

DNP – Delayed Neutron Precursor

DOE – Department of Energy

EFPD – Effective Full Power Days

EHX – Emergency Heat Exchanger

EM – Evaluation Model

EMDAP – Evaluation Model Development and Assessment Process

EOL – End of Life

FHR – Fluoride Salt cooled High Temperature Reactor

FoM – Figure of Merit

FSST- Fuel Salt Storage Tank

GDC – General Design Criteria

HTGR – High Temperature Gas cooled Reactor

IMSR – Integral Molten Salt Reactor

ID – Inner Diameter

IRVACS – Internal Reactor Vessel Auxiliary Cooling System

IrFS – Irradiated Fuel Salt

Keff – k effective

KF – Potassium Fluoride

Kr – Krypton

LEU – Low Enriched Uranium

LWR – Light Water Reactor

MCMC – Markov Chain Monte Carlo

MFS – Makeup Fuel System

MSR – Molten Salt Reactor

MSRE – Molten Salt Reactor Experiment

MSTDB – Molten Salt Thermal Properties Database

MWe – Megawatt electric

MWth – Megawatt thermal

NaF – Sodium Fluoride

NEAMS – Nuclear Energy Modeling and Simulation

NRG – Nuclear Research and Consultancy Group

OD – Outer Diameter

ORNL – Oak Ridge National Laboratory

PHX – Primary Heat Exchanger

PIE – Postulated Initiating Event

PIRT – Phenomena Identification and Ranking Table

PRACS – Process Reactor Auxiliary Cooling System

PSA/PRA – Probabilistic Safety Assessment/Probabilistic Risk Assessment

Pu - Plutonium

RAB – Reactor Auxiliary Building

RG – Regulatory Guide

RV – Reactor Vessel

SCS – Secondary Coolant System

SDA – Standard Design Approval

SDM – Shutdown Mechanism

SS – Stainless Steel

TCS – Tertiary Coolant System

TEI – Terrestrial Energy Inc.

TEUSA – Terrestrial Energy USA

TH – Thermal Hydraulics

UF4 – Uranium Tetrafluoride

UQ – Uncertainty Quantification

Xe - Xenon

Executive Summary

TEUSA's licensing objective is to obtain a Standard Design Approval (SDA) for the IMSR Core-unit. A necessary component of a 10 CFR Part 52 SDA application for the IMSR Core-unit is the identification and description of the radiological source terms that will be used to demonstrate that, in the event of a postulated design basis accident, the regulatory criteria for radiological exposure to the general population will not be exceeded. This white paper summarizes the methodology, key analysis parameters, and generic model of an MSR facility that are important for the generation of a radiological source term that is to be used in calculating the radiological consequences following a postulated design basis accident. The evaluation of radiological consequences following postulated design basis accidents is a necessary element of an application for a license. Any application for a license must demonstrate that the regulatory limits for exposures to the general population of radionuclides released following postulated design basis accidents will not be exceeded. This white paper discusses the key phenomenological attributes of molten fuel salt that contribute to the potential release of volatile radionuclides. This document also discusses key uncertainties that must be considered in estimating a mechanistically derived radionuclide source term. The application of the methodology and simulations specific for the IMSR400 will be described in a future topical report.

I. Purpose

The purpose of this white paper is to describe a broadly applicable, modeling and simulation capability being developed by TEUSA for molten salt reactors (MSRs). The capability will include a methodology for determining and propagating the uncertainties in parameters of importance for fission product source terms specific for MSRs. The capability will be accomplished using the U.S. Department of Energy's (DOE) available Nuclear Energy Advanced Modeling and Simulation (NEAMS) tools. The methodology will be used to predict the radionuclide source term following the design basis event of a break in an off-gas transfer line. The offsite radiological consequences associated with the calculated source term will not be performed in this report. The direct calculation of radionuclides available for potential release from the IMSR will be provided as part of a future topical report.

The elements of this white paper will follow the guidance outlined in Regulatory Guide (RG) 1.203, "Transient and Accident Analysis Methods," December 2005. The specific elements will be discussed in greater detail below in the section on Regulatory Guidance.

II. Introduction

Terrestrial Energy USA, Inc. (TEUSA) is developing the Integral Molten Salt Reactor (IMSR) (also referred to interchangeably herein as the IMSR400) design to provide electricity and/or process heat to U.S. industry. The IMSR is a Generation IV advanced reactor power plant that employs a fluoride MSR design. The reference IMSR nuclear power plant (I-NPP) consists of two Reactor Auxiliary Buildings (RABs) that produce a total of 884 MWth (442 MWth per Core-unit) for 390 MWe (195 MWe per steam turbine) of net electric output. The IMSR400 also has the potential to export 600 °C of heat (from each nuclear island) for industrial applications, or some combination of both heat and electricity. The IMSR400 includes an adjacent steam plant and turbine building for each RAB which contain non-nuclear-grade, industry-standard power equipment.

The IMSR is a thermal spectrum, liquid-fueled, graphite-moderated reactor which is fueled by low-enriched uranium-tetrafluoride (UF_4) dissolved in a fluoride salt-mixture. The fuel salt is a near eutectic mixture of [[ ]], which is the principal heat removal/transfer medium. Fission products with long decay half-lives in the fuel salt build up slowly and over time as the fuel burns up and could be released should a potential design basis accident occur. A variety of radionuclides are formed over the operational lifetime of an IMSR400 plant. However, the volatile isotopic noble gas species of Xenon (Xe) and Krypton (Kr) have special importance both for operational and safety considerations. The noble gas species are created in the core and around the flow loop through direct fission yield or through decay of their respective precursor(s). These noble gas species do not chemically bind with the fuel salt and are highly insoluble in fluoride salt mixtures. Due to their volatility, insolubility, and migration features, some fraction of the noble gas species is expected to diffuse into the graphite moderator structure and transfer out from the free surface of the fuel salt pool into the open gas environment above it.

At present, there is no NRC approved analytical capability for the calculation of source terms following postulated accidents in a MSR. For this reason, TEUSA has partnered with DOE National Laboratories to undertake this generic effort in order to establish an acceptable methodology for calculating source terms mechanistically, including the treatment of uncertainties in phenomenological parameters where specific test data would not be completely available. This generic model could then be used to calculate radiological source terms for any liquid fueled MSR, including the IMSR400.

III. Regulatory Guidance

Regulatory Guide (RG) 1.203 describes a process that the NRC staff considers acceptable for use in developing and assessing Evaluation Models (EMs) that may be used to analyze transient and accident behavior that is within the design basis of a nuclear power plant. While this RG was written to support the review of evaluation models that would be used for light water reactors to demonstrate compliance with 10 CFR 50.46, the process steps laid out in the guidance are directly relevant to the review of an evaluation model for a non-light water reactor.

This regulatory guide is intended to provide guidance for use in developing and assessing evaluation models for accident and transient analyses. Evaluation models that are developed using these guidelines will provide a more reliable framework for risk-informed regulation and a basis for estimating the uncertainty in order to understand transient and accident behavior. To that end, the Discussion section of the RG addresses the fundamental features of transient and accident analysis methods. Furthermore, the Regulatory Position section of the RG describes a multi-step process for developing and assessing evaluation models, and provides guidance on related subjects, such as quality assurance, documentation, general purpose codes, and a graded approach to the process. The Implementation section then specifies the target audience for whom this RG is intended, as well as the extent to which the RG applies. Finally, the Regulatory Analysis section presents the staff's related rationale and conclusion.

To produce a viable product, certain principles should be addressed during the model development and assessment processes. Specifically, the following six basic principles have been identified as important to follow in the process of developing and assessing an EM:

(1) Determine requirements for the evaluation model. The purpose of this principle is to provide focus throughout the evaluation model development and assessment process (EMDAP). An important outcome should be the identification of mathematical modeling methods, components, phenomena, physical processes, and parameters needed to evaluate the event behavior relative to the figures of merit described in the Standard Review Plan and derived from the general design criteria (GDC) in Appendix A to 10 CFR Part 50. The phenomena assessment process is central to ensuring that the EM can appropriately analyze the particular event and that the validation process addresses key phenomena for that event.

(2) Develop an assessment base consistent with the determined requirements. Since an EM can only approximate physical behavior for postulated events, it is important to validate the calculational devices, individually and collectively, using an appropriate assessment base. The database may consist of already existing experiments, or new experiments may be required for model assessment, depending on the results of the requirements determination.

(3) Develop the evaluation model. The calculational devices needed to analyze the events in accordance with the requirements determined in the first principle should be selected or developed. To define an EM for a particular plant and event, it is also necessary to select proper code options, boundary conditions, and temporal and spatial relationships among the component devices.

(4) Assess the adequacy of the evaluation model. Based on the application of the first principle, especially the phenomena importance determination, an assessment should be made regarding the inherent capability of the EM to achieve the desired results relative to the figures of merit derived from the GDC. Some assessment against selected figures of merit can be made during the early phase of code development to minimize the need for later corrective actions. A key feature of the adequacy assessment is the ability of the EM or its component devices to predict appropriate experimental behavior. Once again, the focus should be on the ability to predict key phenomena, as described in the first principle. To a large degree, the calculational devices use collections of models and correlations that are empirical in nature. Therefore, it is important to ensure that they are used within the range of their assessment.

(5) Follow an appropriate quality assurance protocol during the EMDAP. Quality assurance standards, as required in Appendix B to 10 CFR Part 50, are a key feature of the development and assessment processes. When complex computer codes are involved, peer review by independent experts should be an integral part of the quality assurance process.

(6) Provide comprehensive, accurate, up-to-date documentation. This is an obvious requirement for a credible NRC review. It is also clearly needed for the peer review described in the fifth principle. Since the development and assessment process may lead to changes in the importance determination, it is most important that documentation of this activity be developed early and kept current.

The RG describes 19 elements of an evaluation model that are necessary in order that the model can be considered acceptable for use in evaluating postulated accidents. This white paper will follow the guidance elements and discuss each of the 19 elements.

IV. Generic Molten Salt Reactor Design and Accident Scenario Description

IV.1 Overview

For the purposes of developing a generic molten salt reactor modelling and simulation (M&S) capability, a generic design of a potential molten salt reactor design must be developed. [[

]] In addition, for a generic modeling capability to be useable, the generic M&S capabilities must be easily modified to reflect an actual MSR design with the relevant systems and structures that would be present.

Figure 1 shows a schematic layout of a generic MSR design with the Reactor Vessel (RV) inside a shielded Reactor Vault concrete structure. A pictorial representation of the generic RV internals is shown in Figure 2. Figure 3 shows the generic Irradiated Fuel Salt (IrFS) transfer and gas management system which is an integrated system to manage the off-gas and spent fuel. The off-gas that is continuously generated in the RV during normal operation is transferred passively to the Fuel Salt Storage Tank (FSST) through an off-gas transfer line (i.e., the pressure equalization line as shown in Figure 3) that connects the gas space between the operating core-unit and the FSST.

Figure 1. Frontal View of a Generic Molten Salt Reactor

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Figure 2. Schematic of Generic Molten Salt Reactor Internals

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Figure 3. Configuration of Generic Irradiated Fuel Salt and Off Gas Transfer Line

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IV.2 Description of a Generic Molten Salt Reactor Vessel and Internals

The key elements of a generic MSR include the following:

- Reactor Vessel,
- Fuel Salt,
- Primary Pumps,
- Graphite Moderator,
- Primary Heat Exchangers,
- Secondary Coolant System,
- Cover Gas & Off Gas Management System,
- Fuel System,
- Irradiated Fuel System

Descriptions of each of these key elements are provided below.

Reactor Vessel

The RV is an upright, [[ ]] cylinder which contains the full inventory of liquid fuel salt. There are no external fuel salt piping loops associated with the RV. All heat from fission is generated within the RV. [[ ]], the RV forms the primary nuclear boundary during normal operation, anticipated events, and DBAs.

The RV boundary performs the following functions:

- Contains the fuel salt,
- Provides a flow circulation path for the fuel salt, and
- Provides support (anchor point) for the core internals.

The RV itself is a passive boundary. However, instrumentation is used in the RV to measure:

- Temperature,

- Pressure,
- Neutron flux, and
- Fuel salt level.

The RV operates at low pressure and is conservatively designed. A Guard Vessel houses the RV and would catch and contain any leaked fuel salt in the event of a Beyond Design Basis failure of the RV. The Guard Vessel, however, does not form part of the RV.

Liquid Fuel Salt

The MSR modeled for this effort is a thermal spectrum system which operates on the basis of a critical chain reaction caused by fissions of low-assay low enriched uranium (LEU) tetrafluoride (UF_4) dissolved in carrier fluoride salts that together form a combined molten fuel and primary coolant salt mixture. The sustained fission chain reaction and consequent heat generation is primarily conducted by delivery of the salt mixture into a graphite core and subsequent transport to Primary Heat Exchangers (PHXs). The [[

]] over the 7-year operating lifetime of the Core-unit. The lower melting temperature of the fuel salt mixture relative to the operational temperature range implies that the fuel salt mixture will be molten during normal operation. This property, combined with continuous salt transport, ensures uniform distribution of the fuel and fission products throughout the salt volume. Fluoride fuel salt-mixtures offer high potential for nuclear applications as they generally have the following essential characteristics:

- High boiling temperatures;
- Low vapor pressures;
- High heat capacities;
- Low chemical reactivity; and
- High solubility of fission products.

In any potential emergency involving a sudden temperature increase, the core negative temperature reactivity coefficient, owing to the nuclide content and thermophysical properties of the fuel salt-mixture, will inherently stabilize the reactor such that the heat removal systems can passively remove the heat produced.

Using liquid fuel eliminates the need for fuel cladding and high-pressure operation. The fuel salt is expected to behave as a single-phase homogeneous mixture under normal operating conditions and to be radiation hard.

Primary Pumping System

A Pumping System performs the essential function of circulating the fuel salt through the reactor core. Its purpose is to provide enough flow through the PHXs and Moderator to facilitate full power operation without exceeding the material temperature limits of key components.

Such a system could include the pump motor/turbine, couplings, bearings, seals, flow inducer, and pipe connection to the drive (gas or electric) system. It directly [[

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Graphite Moderator

The purpose of the Graphite Moderator is to provide the medium for slowing down neutrons to promote the nuclear chain reaction. The Graphite Moderator core design provides fuel channels for the passage of fuel salt, using pump force, through the moderator region to the PHXs.

Shutdown Rods

A generic molten salt reactor includes an independent means of shutting down the reactor. The means of shutdown would bring the reactor to a sub-critical state, which would eventually result in cooldown to a cold condition as decay heat subsides.

Primary Heat Exchangers (PHX)

The PHXs provide heat transfer between the circulating fuel salt and a separate closed-loop secondary coolant salt. The generic model employs six primary cooling loops (primary pumps and primary heat exchangers). The PHXs receive the fuel salt that has been heated in the reactor core, transfer the heat to the secondary coolant salt, and direct the output fuel salt flow toward the downcomer annulus. The fuel salt then enters the core through the lower plenum of the bottom plate.

A secondary coolant salt circulates on the tube-side of the PHX. This coolant salt transfers the heat away from the reactor core while being isolated from the highly radioactive primary fuel salt liquid.

The PHX design transfers the total core heat load, which is equal to the thermal power produced in the reactor core, plus the additional heat load from the decay heat.

Secondary Coolant System

A generic MSR has a secondary cooling system that delivers heat from the PHX to the Secondary Heat Exchanger where the heat is then transferred to a Tertiary Salt Loop.

Off Gas Management System

A gas space will be present above the fuel salt volume in the generic MSR design. This area facilitates gas expansion, fission gas holdup, and passive cooling while providing means for removal of gaseous fission products during power operation.

Makeup Fuel System (MFS)

The purpose of the MFS is to provide the initial and makeup fuel load for new Core-units and to periodically add fuel to the reactor during operation in order to maintain the reactivity of the core and maintain the fuel temperature at the desired value.

Initial fuel load is “start-up” fuel; fuel added during operations is “make-up” fuel. The system has a safety function to limit the rate and amount of reactivity that can be added to the core in order to ensure that the fuel temperature does not increase in an uncontrolled manner. The system also ensures that fuel outside the reactor cannot go critical.

V. Evaluation Model Development and Assessment Process

V.1 Establish Requirements for Evaluation Model Capability

V.1.1 Regulatory Guide 1.203 Step 1 - Specify Purpose, Transient Class, and Power Plant Class

The first step in establishing evaluation model requirements and capabilities is specifying the purpose of the analysis and identifying the transient class and plant class to be analyzed. The evaluation model is a generic model that can be used for the spectrum of transients and operation that include 1) normal power operation, 2) routine power manipulations, 3) anticipated operational occurrences, 4) postulated DBAs, and 5) some beyond design basis accidents. The model capabilities are to be used for a variety of potential MSRs. However, the applicability of the model will be dependent on the unique characteristics of the relevant MSR design. Any applicant or licensee that would use this generic capability will need to confirm that the model addresses any unique phenomenon specific to the capabilities of their MSR design.

While the M&S capabilities will be initially used for calculating a source term associated with an off-gas transfer line break, the intended use of the methodology by TEUSA is to apply the capabilities to the range of transients and DBAs that are identified for the IMSR400 specifically.

As for application to plant type, the M&S capabilities are specific to pool type MSRs that employ low-enriched uranium as the fuel source. The generic model employs six primary cooling loops (primary pumps and primary heat exchangers). However, the model is not specific only to those primary cooling design characteristics.

The model can be easily modified to reflect the number of primary cooling loops that an alternative MSR design may contain. The model is specific to a graphite moderator for the core region of the MSR. The model is also specific to the use of a fuel salt that does not contain lithium or beryllium. The presence of lithium or beryllium introduces the production of high levels of tritium that are not found in fuel salts that do not contain these elements. Similarly, the generic model employs 6 secondary cooling loops although this number can be modified to reflect the relevant MSR design.

V.1.2 Regulatory Guide 1.203 Step 2 - Specify Figures of Merit (FoM)

Figures of merit are those quantitative standards of acceptance that are used to define acceptable answers for safety analyses. The figures of merit as used here are not to be confused with the term used in the Appendices of this whitepaper. The figures of merit as envisioned by the RG represent the key parameters that are essential to evaluating the overall safety and system performance of a MSR.

For the generic M&S capabilities, important figures of merit for a MSR could be parameters such as fuel salt temperature (no fuel salt boiling), primary system pressure (no energetic release and containment integrity assured), RV material temperatures, temperatures of certain reactor internals such as shutdown rod thimbles (assures capability to insert shutdown rods - dependent on the actual design), reactivity controls (K_{eff} less than 1 during all transient and accident response), heat removal rates (flow rates) for the emergency cooling systems.

These figures of merit are selected because they establish the envelope for integrity of the RV, the ability to take the reactor to a safe state, and assure that no large radioactive releases would occur following design basis events.

The figures of merit listed in the Appendices are for the purpose of ranking by order of importance the various phenomena in order to 1) prioritize actions needed to develop the data that will support future safety analyses and 2) identify areas where the data would not currently exist and would require development of a research and development program.

V.1.3 Regulatory Guide 1.203 Step 3 - Identify Systems, Components, Phases, Geometries, Fields, and Processes That Must Be Modeled

The purpose of this step is to identify the Evaluation Model characteristics. For the generic MSR, the systems and components to be modeled are the components that constitute the primary flow pathway and the structural elements that impact the fuel salt. This would include the graphite moderator, the upper and lower core plates, the flow chimney, the PHX, the secondary cooling pathway, the emergency cooling pathway, the primary salt pumps, the upper head off-gas space, the downcomer annulus, the RV walls, and the shutdown rod thimbles.

V.1.4 Regulatory Guide 1.203 Step 4 - Identify and Rank Key Phenomena and Processes

RG 1.203 states that plant behavior is not equally influenced by all processes and phenomena that occur during a transient. An optimal analysis reduces candidate phenomena to a manageable set by identifying and ranking the phenomena with respect to their influence on figures of merit. The evaluation model development and assessment should be based on a credible and scrutable Phenomena Identification and Ranking Table (PIRT).

At a high level, a PIRT would identify the following key phenomena that would be important to a MSR. The list is not comprehensive but is intended to provide some insights into the factors that would be important in the development and validation of an evaluation model. Some key phenomena are:

1. Removal of fission gases from the fuel salt and effect on reactivity
2. Fuel salt reactivity coefficient
3. Graphite temperature and distortion effects
4. Shutdown mechanism integrity
5. Effect of fission products on reactivity of the fuel salt
6. Impacts of pressure drops through system components on fuel salt flow rates
7. Impacts of radiation heating of RV and internal components
8. Impacts of flow channel sizing on reactivity and heat removal
9. Impacts of bubble entrainment on reactivity and heat transfer.

The information discussed below are assessments that were performed to facilitate the development of the IMSR. The studies reflect a moment in time of the design process. In 2023, Terrestrial Energy Inc. (TEI) initiated an effort to revise and refine the PIRTs for Thermal Hydraulics and Physics to reflect the state of the IMSR design. An important objective of the PIRT process is to systematically identify the available data and determine what additional research and development will be required to support the code accuracy and applicability statements for the safety analyses of the IMSR.

Most of the phenomena from the current TEI PIRTs could be categorized as behaviors, properties, or parameters of interest specific to a PIE analysis category. In the current initiative, the TEI PIRT behaviors, properties, or parameters of interest will be broken down or decomposed to primary or basic phenomena of concern, which remain the same across the PIE categories and safety analysis disciplines. Rationalization in this manner to the lowest level of 'decomposition' and is intended to produce a set of primary phenomena which will facilitate the identification of required validation and test data to support code validation efforts.

When the current effort is complete, the PIRTs listed below will be updated to reflect the associated results.

Thermal Hydraulics PIRT

An initial assessment was performed in 2017. The details of the initial assessment can be found in TEI Assessment Document IMSR400-30800-ASD-002, “IMSR Phenomena Identification and Ranking Tables (PIRTs) Thermal Hydraulic Analysis PIRTs” (Reference 7). As the design evolved, the thermal hydraulic analysis was revisited and revised in 2022 (Reference 8). The details of the PIRT are not described here but can be found in Appendix B to this white paper. A key outcome of the PIRT is the identification of high safety importance – low knowledge areas for molten salt reactor treatment. The table of high safety importance – low knowledge areas are presented here in Table 1. For additional information related to the PIRT, please refer to Reference 8.

Table 1. High Importance – Low knowledge Phenomena

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Reactor Physics PIRT

A reactor physics PIRT assessment was performed in 2019. The details of the ranking assessment are summarized in Appendix A of this report. The actual details of the PIRT assessment can be found in TEI assessment document IMSR400-30500-ASD-012, "IMSR400 Physics Phenomena Identification and Ranking Table" (Reference 9). A key outcome of the PIRT is the identification of high safety importance – low knowledge areas for MSR treatment. The table of high safety importance – low knowledge areas are shown in Table 2. For additional information related to the PIRT, please refer to Reference 9.

Table 2. High Importance – Low knowledge Phenomena

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V.2 Regulatory Guide 1.203 Element 2 - Development of the Assessment Database

Regulatory Guide 1.203 steps 5 through 8 will be developed at a future date and will be included in a future topical report.

V.2.1 Regulatory Guide 1.203 Step 5 - Specify Objectives for Assessment Base

TBD

V 2.2 Regulatory Guide 1.203 Step 6 - Perform Scaling Analysis and Identify Similarity Criteria

TBD

V.2.3 Regulatory Guide 1.203 Step 7 - Identify Existing Data and/or Perform integral Effects Tests and Separate Effects Tests to Complete the Database.

TBD

V.2.4 Regulatory Guide 1.203 Step 8 - Evaluate effects of IET Distortions and SET Scaleup Capability.

TBD

V.2.5 Regulatory Guide 1.203 Step 9 - Determine Experimental Uncertainties as Appropriate

TEUSA, in collaboration with ORNL and ANL, undertook a contractual effort to develop a broadly applicable M&S capability and methodology for the propagation of uncertainties in model parameters of importance to MSR source terms and off-gas systems. This effort resulted in the submittal of a technical report titled "Uncertainty Quantification Methodology for MSR Off-Gas Source Term for the IMSR" (technical report 230512) [Reference 10]. Uncertainties that were addressed in the technical report include those related to nuclear data (e.g., cross sections and yields), the physical properties of the salt (e.g., solubilities and viscosities), thermochemical properties (e.g., vapor pressures), and system design parameters such as power level and fluid flow rates. The developed capability will provide boundary conditions to off-gas systems and will be used for the determination of the source term for postulated radioactive releases important to the licensing analyses.

Off-gas properties/aspects that were included are: [[

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The report referenced above (referred to as the UQ Methodology report or Reference 10) leveraged codes under active development within the Nuclear Energy Advanced Modeling and Simulations (NEAMS) Program at the US Department of Energy (DOE) and the NEAMS Molten Salt Thermal Properties Database (MSTDB). The codes will be presented in a subsequent section of this report. The discussion of uncertainty propagation relies heavily on the work previously submitted.

The equation numbers, table numbers, and variables listed below in the discussion within Section V.2.5 are references to the equations described in much greater detail in the UQ Methodology report referenced above. The equations are not repeated here. Rather, the reader should refer to the UQ Methodology report for a full development of the technical basis. In sum, this report relies on the documentation activities described in the UQ Methodology report.

V.2.5.1. Neutronics and Thermal-Hydraulics Uncertainty Propagation

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V.2.5.2 Chemical Speciation Uncertainty Propagation

For low-volatile gas, Gibbs energy functions are needed to predict the species vapor pres$_{jj}$sures, pp^{gg}, that are used to calculate the gas-liquid interface molar flux, as shown in Eqs. 26 through 29 in Reference 10. For the noble gases (and high-volatility gases such as HF that behave as noble gas), Henry's constants, HH_{jj}, are used in the calculation of the gas-liquid interface molar flux.

An initial sensitivity study will be performed to characterize the nuclides of Reference 10 Table 2 according to volatility and redox potential for the fuel salt composition as a function of core lifetime depletion. The CALPHAD method allows for the effective parameterization of the Gibbs energy function of every phase and species considered in a system. With such description of the mathematical models, changes in phase equilibria and thermodynamic properties of a defined chemical system can be determined as function of temperature, composition, and pressure. Depending on the user's criteria, the implemented models and the number of parameters used to describe the Gibbs energy function of a phase varies. The CALculation of PHAsed Diagram (CALPHAD) methodology will be used to perform thermodynamic predictions of vapor pressures for low volatility fluoride species for the different constituents of the IMSR fuel salt as a function of temperature and composition.

It has been established that deterministic models, where only one set of values for the parameters are considered, have the drawback of not providing any uncertainty bound for actual material design. This issue is found in CALPHAD models where knowledge of the uncertainty of phase boundaries or thermodynamic properties, which are essential for engineering analyses, is not taken into account in the optimization process. Calculations that determine UQ and propagation can better describe the confidence and reliability of thermodynamic models and their predictions.

New tools are available for determining and computing thermodynamic properties that can be used in developing useful UQ methodologies. These include PyCalphad, which is an open-source Python library designed for the calculation of phase diagrams and thermodynamic properties and for the global minimization of Gibbs energy in multicomponent space.

ESPEI is open-source Python-based software developed for automated database development and UQ of parameters. The software provides two fitting modules: single-phase parameter generation and multiphase Markov Chain Monte Carlo (MCMC) simulations. In the multiphase optimization process, MCMC sampling is applied to explore the model parameters that are constrained by experimental or computational data. MCMC calculations numerically sample parameter space to determine parameters for a model that best reproduce the data and therefore result in an understanding of the uncertainty in the parameters.

In an MCMC calculation, a vector (or in ESPEI's terms, a chain) consisting of all the parameters to be assessed in the model is defined. The chain engages in a biased random walk throughout parameter space that after many iterations leads to a reliable best estimate and distribution for each parameter. In a well-defined model, all chains converge to a region of parameter space with the highest posterior probability, which is the probability of reproducing data with the given parameters in the chain. The software defines the optimized parameters as the chain that had the highest posterior probability. With PyCalphad as the minimization engine for open-source optimization in tandem with ESPEI, the opportunity for simultaneous and large-scale UQ, uncertainty propagation, and parameter optimization is possible.

The current proposal intends to implement further additions to the open-source code ESPEI that will allow it to calculate the uncertainty in the gas phase and its properties such as vapor pressure. The present work identifies the three main capabilities that require implementation in ESPEI, modules that 1) automatically calculate the equilibrium partial pressure of species in the gas phase, 2) correctly handle enthalpy and entropy of fusion/vaporization in a chemical system, and 3) improve on parallelization capabilities of the MCMC calculations in available computer clusters. Once these features have been implemented, the project team will determine the size of the chemical system that will be tested with ESPEI. The overall result will allow the rigorous modeling of relevant Gibbs energy functions together with their inherent uncertainty values, allowing the determination of error limits on calculated equilibrium vapor pressures.

V.2.5.3 Uncertainty Propagation in Bulk Liquid- and Vapor-Phase Species Transport

Equations 24 and 25 in Reference 10 represent species transport in the bulk liquid phase and gas phase, respectively, for nuclides defined in Table 1 of Reference 10. For the bulk liquid, [[

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V.2.5.4 DAKOTA UQ Analysis

Table 3 of this report summarizes the physics, model parameter inputs, and calculated QoIs based on the governing equations. [[
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The DAKOTA software from Sandia National Laboratories (Adams et al. 2021) provides a toolbox of advanced parametric analysis techniques enabling quantification of margins and uncertainty, risk analysis, model calibration, and design exploration with computational models. DAKOTA includes methods for optimization, UQ, parameter estimation, and sensitivity analysis, [[
]]

Table 3. UQ analysis model input and output QoIs

[[

]]

Random sampling methods are the “black-box” UQ work horse provided in DAKOTA, as well as the SAMPLER code used with SHIFT. Essentially, [[

]] DAKOTA has several sampling methods, including Monte Carlo and Latin hypercube, that are easy to understand.

V.3 Regulatory Guide 1.203 Element 3 Develop Evaluation Model

V.3.1 Regulatory Guide 1.203 Step 10 Establish an Evaluation Model Development Plan

This report will combine the Regulatory Guide 1.203 development steps 10 through 12 as the evaluation method as described below.

RG 1.203 states that the Evaluation Method structure should include the structure of the individual calculational devices, as well as the structure that combines the devices into the overall evaluation method. The structure for an individual code consists of six ingredients:

(1) Systems and components
(2) Constituents and phases
(3) Field equations
(4) Closure relations
(5) Numerics
(6) Additional features

The following discussion presents the structure of analytical methods used in developing the structure of the evaluation methodology.

Figure 4: A Graphical Depiction of the Evaluation Method

[[

]]

SAM

Code Description: The System Analysis Module (SAM) is a modern system analysis tool under development at Argonne National Laboratory (ANL) and will be used to perform thermal fluid analysis of the primary loop and off-gas system. SAM provides a fast-running, whole plant transient analysis capability with improved-fidelity for advanced non-LWR safety analysis. SAM utilizes an object-oriented application framework (MOOSE) and its underlying libraries to leverage the modern advanced software environments and numerical methods. Currently, the SAM code is being used in many ongoing research and development (R&D) activities to support the thermal-hydraulics (T/H) analysis of different types of advanced non-LWR reactor designs, such as the high temperature gas-cooled reactor (HTGR), fluoride salt-cooled high temperature reactor (FHR), heat pipe-cooled micro-reactor, MSR, etc. NRC has stated its intent to use SAM to perform the safety analyses for the licensing of new advanced reactors. The SAM code is aimed to provide improved-fidelity simulations of transients or accidents in an advanced non-LWR, including three-dimensional resolutions as needed or desired. Multi-dimension, multi-scale, and multi-physics effects can be captured via coupling with other simulation tools, and computational accuracy and efficiency will be state-of-the-art. Uncertainty quantification is integrated into SAM numerical simulations.

The SAM code will include a model of the full primary side of a MSR to simulate the transient behavior of thermal-fluid flow and the associated species and source terms of interest with respect to modeling of a MSR off-gas system. As more physical phenomena regarding the behavior of source term transport in MSR-specific contexts and in the off-gas system design is understood, it is anticipated that some SAM code development will be required to enhance the existing capabilities to model such phenomena or to couple with other analysis tools to perform multi-physics simulation.

Mole

Code Description: Mole is an engineering scale diffusion and reaction kinetics NEAMS developed code that represents the time-dependent species transport into and out of a spatial mesh element within a systems model and is characterized by source and sinks at mesh element interfaces (liquid-solid, liquid-vapor, and thermodynamic driving forces). The sources and sinks include those due to fission and transmutation (requiring coupling to a depletion code such as ORIGEN), flows and advection (requiring coupling to a thermal hydraulics code such as SAM), and chemical state changes (requiring coupling to a thermodynamic data and GEM solver).

The Mole code will be used to determine the species transport throughout the MSR system based on sources and sinks due to advection flows, chemical state changes, and fission and transmutation. For a system geometrical nodalization, the Mole code will be responsible for providing the time-dependent or steady-state composition throughout the system. Mole coupling to SAM will involve receiving the advective flow and temperature (sources and sinks) at mesh boundaries that, with updated thermal conditions, will be used with the MSTDB to update the chemical state. Mole concurrently will use the SHIFT neutronics library to track changes in radionuclides based on flux level and depletion.

Modifications: The modifications to Mole have focused on implementation of additional species transport models to support the off-gas system modeling. Specifically, models are being developed to predict the formation and growth of gas bubbles within the salt, the interactions of other salt species with those bubbles, and the removal of species from the salt by the off-gas system. All changes so far have been restricted to the general chemistry modeling capabilities in the code.

MSR Model: The MSR is modeled in MOLE using one-dimensional geometry. The 1D “pipe” that represents the MSR uses a cross-sectional area that accurately preserves the volume of the salt in the model. This 1D pipe model is set up for the following reactor components: lower head, reactor core (including the graphite moderator), pumps, chimney, upper head, heat exchangers, and the downcomer. The 1D model is a closed loop so that salt exiting the end of the downcomer reenters the inlet of the lower head. MOLE has been coupled to GRIFFIN for this model to track delayed neutron precursors in the flow fuel salt. The GRIFFIN calculations use cross sections generated by SHIFT to calculate the power distribution, while MOLE uses that power distribution to calculate the source terms for delayed neutron precursors and other important nuclides.

SHIFT

Code Description: SHIFT is a parallel, Monte Carlo solver for radiation transport application development on high-performance computing (HPC) platforms with multiple physics and geometry options. SHIFT is integrated with the Denovo deterministic solvers for hybrid radiation transport calculations and can execute on CPU and GPU based architectures. Applications of SHIFT include LWR and non-LWR reactor analysis and design, radiation shielding, criticality safety, radiation dosimetry, and fusion system analysis. SHIFT supports two-step workflows to pre-generate cross sections for given temperature and density distributions, and ex-core detector or dose assessment. SHIFT is integrated with ORIGEN for depletion and SAMPLER for cross section uncertainty analysis as part of the SCALE system.

The SHIFT Monte Carlo code, which solves for the neutron flux, based on continuous neutron energy and generalized geometry will be used to determine the reaction rates for the specific MSR design. The reaction rates form the basis of production/destruction rates for all nuclides within the liquid-fuel inventory as well as the power level of the reactor. The SHIFT code coupled with ORIGEN for nuclide transmutation and fuel depletion will be used to provide the neutronic source and sink term for the

Mole code. This will also serve as the calculation for decay heat based on the nuclide composition of the reactor. This will need to be a function of the operating history of the reactor. In addition, SHIFT will be used to provide kinetics parameters to the SAM code. As part of this development, uncertainties in nuclear data and their impact on nuclide composition will be assessed and will form the basis for later UQ analysis relevant to source term.

The SHIFT model developed will be used to generate a database of nuclide transmutation data as a function of salt burnup that can later be used in standalone ORIGEN simulations to provide isotopic source and sink terms to Mole. The SAMPLER code, which is part of the SCALE package (along with SHIFT), will be used to perturb the underlying nuclear data in the continuous energy libraries to provide a set of transmutations libraries that can be randomly sampled to represent the variation in nuclear data specific to the IMSR reference model which will ultimately be a source of uncertainty that will propagate to the off-gas system.

The SHIFT model will also be used to compute point kinetics parameters that will be used in SAM for a range of operational transients and accident scenarios to establish the load that will be placed on the off-gas system in off-nominal conditions. In a similar way, the SAMPLER package will be used to establish a set of point kinetics parameters that vary because of uncertainty in the underlying nuclear data.

For the uncertainties in the nuclear data, the SAMPLER sequence of the SCALE code system allows for random sampling-based uncertainty analysis with respect to uncertainties in the nuclear data to be fed in directly to SHIFT. In addition, SAMPLER allows for the identification of nuclide reactions that are significant contributors to the uncertainty in output quantities of interest. Within the SAMPLER approach, cross sections are perturbed based on the uncertainty and correlation information given in the corresponding nuclear cross section covariance matrices.

A detailed 3-dimensional core was modeled, including the heat exchanger, pump, and vessel as seen in Figure 5.

Figure. 5. Generic MSR SHIFT Model

[[

]]

To simulate the fuel cycle of an MSR, Shift from the SCALE front end was used since it has the feature to do the continuous nuclide feed and removal. In the depletion, a time step of 7 days was chosen. Noble gases and metals are continuously removed. However, the postulated MSR adopts a makeup fuel feed mechanism that allows for the vessel's growing volume of fuel salt. Therefore, the continuous feed feature in the code cannot be used. However, the feed simulation was performed by an external script to call ORIGEN to blend the irradiated and fresh fuel salt, and the blended mixture is the composition for the next depletion time step.

Molten Salt Thermal Properties Database (MSTDB)

Description: Fundamental to radionuclide tracking, in general, are thermophysical and thermochemical properties. These are generated using ab initio and classical molecular dynamics simulations and curated into reduced order empirical relations for the thermophysical properties. The CALPHAD approach is used for the thermodynamic assessments. The development continues to extend the MSTDB to include all the elements that will exist during operation of a MSR to model the thermal properties with burnup along with additives and corrosion products.

Application: To address the uncertainties in the molten salt properties, the evaluation method leveraged the NEAMS MSTDB which is a collection of models and associated parameters for representing the thermodynamics and thermophysical behavior of molten salts with burnup including additives and corrosion products. The thermochemical outputs relevant to this proposed project are vapor pressures of volatile species, examples of which include Cesium-Iodine (CsI) and other Iodine-bearing gas phase constituents. Thermophysical properties impact the thermal hydraulic behavior of a reactor. As such, the outputs to be used in the proposed multi-physics modeling framework are density (ρ), viscosity (ν), thermal conductivity (κ), and specific heat or heat capacity (Cp).

The MSTDB uncertainties originate from the experimental measurements or computational inputs used to optimize the model parameters. The thermophysical properties are empirical relations making error propagation straightforward. This task will determine the uncertainty in the MSTDB thermophysical properties outputs resulting from the data used to optimize the adjustable parameters of the thermodynamic models using error propagation strategies.

V.4 Regulatory Guide 1.203 Assess Evaluation Model Adequacy

This report will address the combination of Regulatory Guide 1.203 Steps 13 through Step 18 in an integrated way. These steps describe the physical models used and the incorporation of actual data into the models. The results of the calculations from the model are evaluated against physical data or other computer simulations to determine if the evaluation model is properly predicting the results.

V.4.1 The Molten Salt Reactor Model

In order to demonstrate the capabilities of the evaluation method, it is necessary to describe and define the system to be evaluated and the parameters of that system that are essential elements of the analysis. For the purposes of this report, the molten salt reactor that is being used for the modeling and simulation efforts is a hypothetical design that may be reflective of [[ ]] Reactor. The information provided in Section V.4 is a high-level discussion of the detailed analysis of a [[ ]] The details provide context of the parameters and characteristics of the [[ ]] using the NEAMS platform of codes. The dimensions of the [[ ]] The actual dimensions provided in this section reflect the dimensions that were integrated into the NEAMS codes. However, the actual modeling of the various Core-unit components was adjusted to reflect the unique modeling capabilities of the NEAMS codes, so the modeling and simulations were not exactly one-to-one. The details of the modeling differences will be discussed in Section V.5 below.

[[ ]] was the availability of analytical simulations of the system that could be used as a reference for the demonstration that the NEAMS methodologies was accurately predicting the behavior of key elements of a MSR design.

The power and heating properties of this version of the reactor were assessed using models built in MCNP and Flownex. Importantly, power deposition values obtained from the MCNP analyses were used as inputs to the Flownex simulations. Thorough descriptions of both the MCNP and Flownex inputs and outputs are detailed in Section V.4.1. Note that the reactor assessment also accounted for a chimney structure, pump inlet pipes, and IRVACS removal rate performance curves. An illustration of this early reactor version is given in Figure 6.

The reference document for the details of the modelling which includes the working equations and the results is TEI document, IMSR400-30200-ASD-042.45," Flownex Simulation Model for CoreE1_t using MCNP data." [Reference 2]. This referenced TEI document will be provided to inform the NRC review as it relates to the development of important design parameters that are essential inputs to the NEAMS codes. Some specific parameters are copied into the whitepaper for ease of reference. Equations and nodalization details are retained in the reference document.

V.4.2 The System Model

The MSR used to demonstrate the capabilities of the evaluation model is a [[
]]. The [[

]] are shown in Figures 6 and 7.

Figure 6. Components inside the Reactor Vessel (RV)

[[

]]

Figure 7. Top View of the Core Section

[[

]]

Table 4. Graphite Core Parameters

[[

]]

For the Flownex model, each channel ring is [[

]] as shown in Table 5.

Table 5. Channel Ring Data for the Core

[[

]]

The reactor core is modeled in [[

]]

During operation, the power gets deposited in the entire primary system. The power distribution obtained from [[ ]] only. In order to simulate a realistic temperature distribution in the core and all out-of-core components during normal operation, a detailed power distribution is required for all components within the primary system. The [[

]] are used as inputs.

Table 6. Power distribution from MCNP calculations (Reference 2)

[[

]]

In addition to the reactor core, the components modeled within [[ ]] are shown in Figure 8. The dimensions of these components are given in Table 7.

Figure 8. Chimney and Downcomer Locations

[[

]]

Table 7. Component Dimensions

[[

]]

Boundary Conditions

For the steady state calculations, the top free-liquid surface of the fuel salt is kept [[
]]

Modeling Assumptions

[[

]]

Reactor Core Model

As shown in Figure 2, the graphite core contains [[

]]

Flow through channels inside the graphite core

As shown in the Table 3, there are three different fuel salt [[

]] to fuel salt flow. Therefore, fuel salt flow rates [[

]] are used in the Flownex

model to represent [[
]] rings.

Distribution of power across different components of the Reactor Vessel

The power obtained from the [[
]] components. Table 8 shows the power at various locations in the Flownex model for the IMSR400 and the corresponding components where they are deposited.

Table 8: Distribution of Power Obtained from MCNP to Different Components.

[[

]]

Distribution of power in channel rings and graphite

The MCNP simulations of the [[

]] are utilized for this purpose.

Primary Heat Exchanger Design

The primary heat exchanger is a [[ ]] (See Figure 9). PHX modeling parameters are given in Table

Figure 9. PHX design

[[

]]

Table 9. PHX parameters

[[

]]

Salt Thermo-Physical Properties

The thermo-physical properties of the fuel salt in Table 10 are taken from [Reference 14]. The highlighted values in the table are taken [[

]]

normal operation conditions.

Table 10. Thermo-Physical Properties of Fuel Salt

[[

]]

The thermophysical properties of the Coolant Salt in Table 11 are taken from [Reference 15].

Table 11. Experimental Melting Point and Experimental and Calculated Thermo-Physical Properties of [[ ]]

[[

]]

Graphite Thermo-Physical Properties

Three different grades of graphite are pre-selected for Graphite Irradiation Assessment Program by TEI. The thermal conductivity and heat capacity of each of the graphite grades [Reference 16] at BOL are shown in Table 12 Graphite Thermo-Physical properties at BOL.

Table 12. Graphite Thermo-Physical properties at BOL

[[

]]

The graphite grade with [[ ]]. This is a conservative choice. Conductivity values are only measured and listed up to 800 C for these graphite grades. For simulation purposes, the 800 C values are used at 1000 C.

Sufficient data was not available for any of the [[

]]

Table 13. Graphite Thermo-Physical properties at EOL

[[

]]

Other Material Properties

Other materials used in the model are listed in Table 14. These properties are taken from the Flownex Database and other sources.

Table 14. Material Properties for RV wall, thimbles, and shield

[[

]]

Distribution of power in reflectors, shield and thimbles

The graphite moderator is [[

]]

The [[

]] simulations.

These powers are [[ ]]

Modeling of the fuel salt flow through the PHX

The fuel salt flows [[

]]

The fuel salt is pumped into [[

]] The secondary coolant salt flows through [[

.]]

Modeling of fuel salt flow through downcomer

The fuel salt flows [[

]]

VI. Modelling Using the NEAMS Codes

This section describes the variations and different modelling assumptions used in establishing the MSR models. [[

]]

VI.1 Code Modeling Modifications

VI.1.1 Reactor Core Model

[[

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VII. Discussion of Results from the Modelling and Simulation Activities using the NEAMS Codes

[[

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Appendix A: Discussion of the PIRT activities related to Core Physics

General PIRT Process Description

The PIRT process used in NGNP (Next Generation Nuclear Plant) PIRT (NUREG/CR-6944) was adopted for the IMSR400 thermal-hydraulic PIRT tables. [[

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Appendix B: Discussion of the PIRT activities related to Thermal Hydraulics

PIRT Process

The development of the PIRT document is an iterative process and the document will be revised as the design of the IMSR400 evolves. [[

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