Regulatory Technology Development Plan Sodium Fast Reactor

Mechanistic Source Term – Trial Calculation

Nuclear Engineering Division

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Regulatory Technology Development Plan

Sodium Fast Reactor

Mechanistic Source Term – Trial Calculation

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Executive Summary

The potential release of radioactive material during a plant incident, referred to as the source term, is a vital design metric and will be a major focus of advanced reactor licensing. The U.S. Nuclear Regulatory Commission has stated an expectation for advanced reactor vendors to present a mechanistic assessment of the potential source term in their license applications. The mechanistic source term presents an opportunity for vendors to realistically assess the radiological consequences of an incident and may allow reduced emergency planning zones and smaller plant sites. However, the development of a mechanistic source term for advanced reactors is not without challenges, as there are often numerous phenomena impacting the transportation and retention of radionuclides.

This project sought to evaluate U.S. capabilities regarding the mechanistic assessment of radionuclide release from core damage incidents at metal fueled, pool-type sodium fast reactors (SFRs). The purpose of the analysis was to identify, and prioritize, any gaps regarding computational tools or data necessary for the modeling of radionuclide transport and retention phenomena. To accomplish this task, a parallel-path analysis approach was utilized, as shown below. One path, led by Argonne and Sandia National Laboratories, sought to perform a mechanistic source term assessment using available codes, data, and models, with the goal to identify gaps in the current knowledge base. The second path, performed by an independent contractor, performed sensitivity analyses to determine the importance of particular radionuclides and transport phenomena in regards to offsite consequences. The results of the two pathways were combined to prioritize gaps in current capabilities.

The primary conclusion of this project is that a mechanistic assessment of radionuclide release from a pool-type, metal fuel SFR core damage incident is possible utilizing current tools and data, with certain limitations. Gaps in models and data regarding some phenomena result in uncertainties, or the use of conservative assumptions, which could make the process of justifying reduced emergency planning zones or plant sites difficult for vendors and also potentially impact design decisions that are dependent on realistic source term analyses.

Specifically, three major gap areas dominated the mechanistic source term assessment:

- 1) **Bubble Transport** – There are large uncertainties regarding the transport of radionuclides within bubbles in the sodium pool. This pathway could result in a bypass mechanism for radionuclides that would otherwise be largely retained within the sodium pool. Properly characterizing the bubble pathway is essential to a realistic source term assessment, but data and tools in this area

are lacking. Gap closure in this area could be accomplished through experiments with non-radioactive elements.

- 2) **In-pin Migration and Release** – Due to insufficient data regarding the migration of radionuclides within the fuel pin and subsequent release during fuel pin failure (as described in more detail in ANL-ART-38), bounding radionuclide release fractions from failed fuel pins are necessary. These assumptions impact subsequent steps of the analysis and may produce potentially unrealistic results, such as comparatively large releases of transuranics. Gap closure regarding radionuclide release during fuel pin failure is difficult, but further work to characterize in-pin radionuclide migration is less challenging and currently possible.
- 3) **Aerosol Behavior** – The accurate modeling of radionuclide behavior within the cover gas region and containment can be problematic due to the unique chemical forms and interactions associated with SFR radionuclide (and sodium) release. Although conservative assumptions are straightforward to apply regarding selected phenomenological gaps, such as aerosol deposition, other phenomena, such as chemical interactions, are more difficult to address through gross assumptions.

Utilizing the findings of the sensitivity study, the gaps identified during the mechanistic source term analysis were prioritized. In addition, recommendations for future research were developed based on specific aspects of the phenomena gaps. These recommendations (listed below in order of “gap group” prioritization) would significantly reduce the uncertainties noted during the mechanistic source term calculation, and provide a more accurate source term assessment for use during future SFR design efforts and license applications.

Recommendations for Future Research

Gap Group	Recommendations
<i>Bubble Transport</i>	<ul style="list-style-type: none"> • Formal completion of the IFR bubble code, including development of documentation and code licensing pathway. • Experimentation regarding failed fuel pin blowdown and entrainment of released radionuclides in bubble (cross-cutting research with reactivity effects of channel voiding and structural impacts of failed fuel pin blowdown on neighboring fuel pins). • Experimentation regarding removal of radionuclides from bubble traveling through sodium pool.
<i>In-Pin Migration and Release</i>	<ul style="list-style-type: none"> • Continued metal fuel PIE to determine radionuclide migration within fuel pin during irradiation. • Experimentation regarding radionuclide release from failed high burnup fuel pins at high temperatures (above fuel melting point) in liquid sodium.
<i>Aerosol Behavior</i>	<ul style="list-style-type: none"> • Continued development of SFR version of MELCOR. • Assessment of available data regarding deposition/condensation/chemical interactions within cover gas region and containment.
<i>Hold-up/Leakage</i>	<ul style="list-style-type: none"> • Response of reactor head seals during transient conditions.
<i>Vaporization</i>	<ul style="list-style-type: none"> • Investigation of non-homogeneous mixing of radionuclides in liquid sodium.
<i>Dispersion</i>	<ul style="list-style-type: none"> • Assessment of applicability of dose conversion factors and deposition assumptions to chemical and physical radionuclide forms likely in SFR radionuclide release.

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Acronyms

Argonne	Argonne National Laboratory
CRBRP	Clinch River Breeder Reactor Program
DF	Decontamination Factor
DOE	U.S. Department of Energy
DRACS	Direct Reactor Auxiliary Cooling System
EBR-II	Experimental Breeder Reactor II
EPA	U.S. Environmental Protection Agency
FFTF	Fast Flux Test Facility
FY	Fiscal Year
HEDL	Hanford Engineering Development Laboratory
IFR	Integral Fast Reactor
KAERI	Korean Atomic Energy Research Institute
LWR	Light Water Reactor
MOI	Maximally Exposed Offsite Individual
MST	Mechanistic Source Term
NRC	U.S. Nuclear Regulatory Commission
PIE	Post-Irradiation Examination
PLOF+	Protected Loss of Flow Scenario
PWR	Pressurized Water Reactor
RTDP	Reactor Technology Development Plan
SAR	Safety Analysis Report
SFR	Sodium-cooled Fast Reactor
SNL	Sandia National Laboratories
SOARCA	State-of-the-Art Reactor Consequence Analysis
SRT	Simplified Radionuclide Transport (Code)
STCP	Source Term Code Package
TEDE	Total Effective Dose Equivalent
TREAT	Transient Reactor Test Facility
UTOP+	Unprotected Transient Overpower Scenario

1 Introduction

The U.S. Nuclear Regulatory Commission licenses and regulates the Nation's civilian use of radioactive materials to protect public health and safety, promote the common defense and security, and protect the environment.

- U.S. Nuclear Regulatory Commission Mission Statement

As stated above, the primary mission of the U.S. Nuclear Regulatory Commission (NRC) is the protection of the public and environment from the accidental release of radioactivity. With this in mind, it is not surprising that there is such strong emphasis on the potential release of radioactivity (the source term) during the NRC reactor licensing process. While the current light-water reactor fleet was licensed through the use of conservative, bounding source term analyses, the NRC has repeatedly indicated an expectation that future advanced reactors license applications will include a mechanistic assessment of potential radionuclide releases [1-3]. While the use of realistic source term assessment models provides advanced reactor vendors the opportunity to potentially reduce emergency planning zones and the size of plant sites, properly accounting for the multitude of possible radionuclides transport and retention phenomena is a challenging task. In addition, the ability to perform a realistic source term assessment is a vital tool during the reactor design process, as it promotes the use of risk-informed design decisions.

Since the successful operation of the EBR-II experimental reactor program, it has been apparent that a metal fueled, sodium-cooled fast reactor (SFR) has a number of safety and performance characteristics that make it an attractive candidate as an advanced reactor concept. Currently, there are multiple U.S. industry vendors proposing metal fueled, pool-type SFR designs. As part of a project to identify and address potential future impediments to SFR licensing, an effort was established to characterize the U.S. capabilities for the mechanistic assessment of radionuclide release following a core damage incident at a metal fueled, pool-type SFR. The goal of this work was to identify and prioritize gaps in the current computational capabilities, and the associated knowledge base, regarding the mechanistic assessment of an SFR source term.

Key Project Point

The goal of this project is to identify and prioritize gaps in current computational capabilities, and the associated knowledge base, regarding the mechanistic assessment of an SFR source term.

1.1 Background

Beginning in FY14, under the auspices of the U.S. Department of Energy (DOE) Regulatory Technology Development Plan (RTDP), Argonne National Laboratory (Argonne) initiated a study of possible impediments to the licensing of an SFR in the U.S.¹ The issues highlighted by this study included the selection of licensing basis events, the regulatory treatment of sodium fires, and the certification of seismic isolators, amongst others. However, only one topic, the development of a mechanistic source term (MST), was found to have both high regulatory importance and a possible “long” lead-time to resolution. Therefore, this issue was selected for further investigation under the RTDP.

Research regarding the development of an SFR MST began in early FY15 with the Argonne report ANL-ART-3 [5]. As shown in the MST developmental pathway in Figure 1-1, ANL-ART-3 sought to identify and characterize radionuclide sources within the reactor, and identify and characterize radionuclide transport and retention phenomena. The report documented these findings through a series of relational

¹ This work was preceded by a Sandia National Laboratories (SNL) study of SFR licensing issues [4].

diagrams, like the one shown in Figure 1-2 for a core damage accident. In addition, ANL-ART-3 also reviewed past accidents and experiments related to the current knowledge base, and performed a preliminary gaps analysis.

Figure 1-1: MST Development Pathway with Associated Reports

Figure 1-2: SFR Core Damage Accident - Radionuclide Transport and Retention Phenomena [5]

Among the findings of ANL-ART-3, two noted gaps were selected for follow-on work in FY16:

- 1) ***Metal Fuel Radionuclide Release Fractions*** – ANL-ART-3 noted that it was unclear whether sufficient data and experience existed to develop radionuclide release fractions from failed metal fuel pins to the primary sodium.
- 2) ***Trial MST Calculation*** – ANL-ART-3 noted that no single, comprehensive computer code existed for an SFR MST. Instead, there were several computational tools that could analyze separate parts of the calculation. It was recommended to conduct a trial MST to determine the sufficiency of this approach and the adequacy of the related computational tools.

The first gap was explored in ANL-ART-38 [6], which conducted a review of metal fuel data and determined radionuclide release fractions from failed metal fuel to the primary sodium under a variety of temperature conditions. The second gap, regarding MST computational tools and the need for a trial MST calculation is explored in detail here.

1.2 Methodology and Report Structure

As stated at the beginning of this section, the goal of the trial MST calculation is to gauge the adequacy of current computational tools and the associated knowledge base for the assessment of an SFR MST. To accomplish this goal, a parallel-path analysis methodology was developed. As shown in Figure 1-3, the methodology consists of both an MST calculation and a simplified source term sensitivity analysis. The MST calculation uses best-estimate codes and models in an attempt to realistically assess the transport and release of radionuclides. The goal of this analysis pathway is to identify any gaps in current computational capabilities or the associated knowledge base. The sensitivity calculation uses simplified radionuclide transport and retention models to conduct a parametric evaluation. The purpose of the sensitivity calculation is to rank transport and retention phenomena in terms of their importance on offsite consequences (offsite dose and land contamination). There were several reasons for the decision to conduct a separate sensitivity calculation. First, simplified models were more conducive to parametric evaluations than the mechanistic models, some of which were time consuming to utilize. Second, an independent contractor was selected to perform the sensitivity calculation, in an effort to assure possible biases in the MST calculation would not influence the ranking of phenomena.

Figure 1-3: Project Methodology

The report structure follows that of the analysis methodology, as shown in Figure 1-4. Section 2 provides an overview of the trial MST calculation, including the models and data utilized and identified gaps.

Section 3 contains an overview of the sensitivity analysis, noting those isotopes and transport/retention phenomena of highest importance to offsite consequence. Finally, Section 4 prioritizes the gaps found in the trial MST in Section 2, using the insights from the sensitivity analysis in Section 3.

Figure 1-4: Report Outline

2 Trial Mechanistic Source Term Calculation

The purpose of the trial MST calculation was to utilize current modeling tools, and the associated knowledge base, in a comprehensive test of their adequacy in performing a complete SFR MST analysis. However, to properly gauge the suitability of the data and tools for the future licensing of SFRs, the trial MST had to include several key characteristics:

- 1) The trial MST must attempt to account for all pertinent radionuclide transport/retention phenomena regarding SFR core damage incidents. This includes exercising available tools and data. If it is determined to not be possible to model a phenomenon, the gap should be noted and analysis assumptions may be made to allow the MST calculation to proceed.
- 2) The modeling tools should be comparable to those traditionally used in nuclear safety analyses (*i.e.*, the computational tools should not require extreme computing capabilities, such as super computers, and execution times must be reasonable, to allow for uncertainty quantification).
- 3) The reactor design analyzed must be prototypic of those currently proposed by the SFR industry, with an emphasis on maintaining consistency of the radionuclide barriers and transport/retention phenomena.

The first key characteristic, regarding the modeling of radionuclide transport/retention phenomena, will be discussed in detail in each of the following subsections. At the end of each subsection, there is a table discussing the phenomena modeled during that analysis step, as shown in the example Table 2-1. The table notes the phenomenon considered, how it was modeled, whether there was a gap identified, and finally if a gap was noted, the resulting impact on the trial MST calculation. This information is used in Section 4 (in conjunction with the Section 3 sensitivity analysis) to rank the identified gaps and prioritize future research. Also, as will be described in Section 2.2, assessing models and data associated with all pertinent phenomena was particularly challenging and resulted in the inclusion of two separate transient analyses.

Table 2-1: Phenomena Overview – Example Table

Phenomena	Modeling	Gap?	Impact on MST Trial
<i>Transport/retention phenomenon considered</i>	<i>Modeling tool used in MST trial calculation</i>	<i>Was a gap identified? (No, Yes, Partial)</i>	<i>If a gap was identified, what was the impact on the MST trial calculation (i.e., a conservative assumption was used in place of mechanistic modeling).</i>

The modeling of transport/retention phenomena also highlights the potential confusion regarding the meaning of “mechanistic.” In some industries, mechanistic modeling is taken to represent models based on first-principles, such as physics-based rather than data-driven models. In SECY-93-092 [1], the NRC defined the characteristics of an MST by the following:

A mechanistic source term is the result of an analysis of fission product release based on the amount of cladding damage, fuel damage, and core damage resulting from the specific accident sequences being evaluated. It is developed using best-estimate phenomenological models of the transport of the fission products from the fuel through the reactor coolant system, through all holdup volumes and barriers, taking into account mitigation features, and finally, into the environs.

- SECY-93-092

For the analysis conducted here, the NRC MST definition is interpreted to imply that phenomena are represented as realistically as possible, using any available models, whether physics-based or data-driven.

The second key characteristic highlights the type of modeling tools employed. Computational tools exist that simulate chemical interactions on the atomic-scale, and computational fluid dynamics could model primary sodium flow conditions in 3-D. However, utilizing such programs for an MST assessment would

require extreme computational capabilities (and validating such high-fidelity codes could pose an additional challenge for future licensing efforts). Therefore, the tools used for the trial MST should be comparable to those traditionally used in nuclear safety analyses.

The third key characteristic, regarding consistency with industry SFR designs, is discussed in detail in Section 2.1.

2.1 Reference Reactor and Calculation Overview

2.1.1 Reference Reactor

As described at the beginning of this section, one of the prerequisites for the trial MST calculation was to maintain consistency with industry SFR designs, particularly the radionuclide barriers. Table 2-2 provides an overview of U.S. SFR vendor reactor designs. All three U.S. vendors utilize metal fuel, pool-type designs. Both burners and breed/burn designs have been proposed. Generally, the radionuclide barriers are the same across all three designs (fuel matrix, cladding, primary sodium, primary system boundary, containment). However, vented fuel concepts have been discussed, which would signify a deviation from historic U.S. SFR designs².

Table 2-2: U.S. SFR Vendor Design Characteristics

Parameter	TWR-P	PRISM	ARC-100
<i>Reactor Power</i>	1475 MWth/500 MWe	840MWth/311 MWe	260 MWth/100 MWe
<i>Type</i>	Pool-type	Pool-type	Pool-type
<i>Purpose</i>	Breed and Burn	Burner	
<i>Core Fuel</i>	U-Zr	U-Zr/U-Pu-Zr	U-Zr
<i>Primary Coolant - Inlet/Outlet (°C)</i>	360/500	360/500	355/510

A reference reactor design was selected that is representative of the designs currently being proposed by the SFR industry. A 1000 MWth (380MWe) pool-type SFR design was selected, with the characteristics shown in Table 2-3, which was based on previous Argonne SFR design concepts. An SFR design larger than some industry concepts was purposefully selected to ensure an accurate investigation of source term phenomena. A very small SFR may have an insignificant potential source term, which could lead to the dismissal of phenomenological uncertainties that could be significant for the safety analysis of a larger reactor. The reference reactor uses a sodium-bonded ternary U-Pu-Zr fuel, separated into three core fuel batches. The reference design is an actinide burner (the sensitivity study reviewed in Section 3 examines the impact of the use of a breeder core).

Table 2-3: Reference Reactor Properties

Parameter	Description
<i>Reactor Power</i>	1000 MWth/380 MWe
<i>Type</i>	Pool-type
<i>Purpose</i>	Actinide Burner
<i>Core Fuel</i>	U-Pu-Zr
<i>Cladding Material</i>	HT-9
<i>Core Fuel Batches</i>	3
<i>Primary Coolant Temp – Inlet/Outlet</i>	350°/500°C
<i>Number of Fuel Assemblies</i>	180
<i>Fuel Pins per Assembly</i>	271

As shown in Figure 2-1, the fuel pins of the reference reactor are slightly over three meters in length, with a fission gas plenum approximately one and a half times the length of the active fuel. The U-Pu-Zr is surrounded by a sodium bond, which maintains thermal contact with the HT-9 cladding when the fuel is at low burnup. The three fuel batches, described in Table 2-4, are assumed to have burnup levels at ~2%, 5%, and 10%. A simplified schematic of the reactor vessel layout is shown in Figure 2-2. The reference reactor utilizes a DRACS emergency decay heat removal system. Detailed properties regarding the reactor system, which will be utilized in subsequent sections, are presented in Table 2-5. The reactor containment, described in Table 2-6, is similar to that of a large-dry PWR containment, but on a smaller scale.

² Vented fuel has been used internationally in liquid metal fast reactors, such as the Dounreay Fast Reactor in the UK.

Figure 2-1: Reference Reactor Fuel Pin Diagram

Table 2-4: Reference Reactor Fuel Batch Description

Parameter	Batch A	Batch B	Batch C
Number of Assemblies	60	60	60
Burnup - at%	~2%	~5%	~10%
Internal Pressure – MPa (psi) ¹	0.51 (74)	3.00 (435)	6.74 (977)

¹At normal operating temperatures

Table 2-5: Reference Reactor System Properties

Parameter	Description
Volume of Hot Pool	756m ³
Volume of Cover Gas	166m ³
Nominal Sodium Depth to Top of Active Core ¹	6.045m

¹At normal operating temperatures and flow

Table 2-6: Reference Reactor Containment Properties

Parameter	Description
Volume	8000m ³
Design Basis Leak Rate	1.0% Vol/Day

Figure 2-2: Reference Reactor Simplified Layout

2.1.2 Trial MST Calculation Overview

The trial MST calculation involves numerous analysis steps, with each step including multiple sub-analyses. Figure 2-3 presents a graphical overview of the MST trial calculation. To aid the reader in following the calculation process, symbols for each calculation step are present at the bottom of the following pages, which highlight the step of the analysis currently under examination.

Figure 2-3: Trial MST – Calculation Process

The trial MST calculation begins with the modeling of the transient scenario. This is followed by the determination of the in-pin radionuclide distribution prior to fuel pin failure. Next is the analysis of radionuclide release post-fuel pin failure. Bubble transport through the sodium pool follows fuel pin failure, along with radionuclide release from the sodium pool to the cover gas region. Analyses of radionuclide behavior in the cover gas region and containment are next, with the final step being offsite radionuclide dispersion.

The trial MST calculation was conducted through a collaboration between Argonne and Sandia National Laboratories (SNL). As shown in Figure 2-4, Argonne performed the initial five steps of the analysis, to the point of radionuclide release to the cover gas region. From there, the analysis split (as will be described in Section 2.7), with SNL leading an analysis of radionuclide behavior in the cover gas region and

containment utilizing a developmental version of CONTAIN-LMR, while Argonne conducted a similar analysis using a surrogate computer code.

Figure 2-4: Trial MST – Division of Analysis

Each of the following subsections provide a summary of the calculation steps. The subsections begin with an overview of the phenomena involved and the methodology utilized to model the phenomena. This is followed by two further subsections that describe the application of the methodology for the two transient scenarios under consideration. As mentioned previously, each subsection ends with a summary of the phenomena modeled, including the identification of gaps.

2.2 Transient Scenario Modeling

As stated in the MST analysis requirements at the beginning of this section, it was desired to model SFR transient scenarios that involved all pertinent source term phenomena related to SFR core damage transients. However, there were some phenomena that were mutually exclusive to certain types of transients. Therefore, two reactor transient scenarios were selected for the MST calculation. These scenarios represent two distinct types of SFR core damage transients. One scenario with prolonged elevated core temperatures, which results in fuel pin failures without fuel melting, and another scenario with a rapid rise in fuel temperatures resulting in fuel melting but with the remainder of the primary system at near-nominal conditions.

Key Project Point

It was necessary to select two transient scenarios to encompass all relevant radionuclide transport/retention phenomena. The two transient scenarios were chosen to provide the desired core damage conditions, and their selection should not be misconstrued as an indication of their specific importance to future SFR licensing efforts.

Protected Loss of Flow (and Heat Sink) with Degraded Decay Heat Removal

- PLOF+
- Slow rise of core temperatures
- Pin failures due to eutectic penetration with no bulk fuel melting
- Very high primary system temperatures

Severe Unprotected Transient Overpower

- UTOP+
- Rapid rise in core temperatures
- Fuel melting resulting in pin failures
- Near-nominal primary system conditions

Phenomena related to extremely unlikely metal fuel SFR transients, such as core disruption accidents (core energetics) or double vessel failure with loss of primary sodium, were excluded from the trial MST calculation. It is assumed that SFR vendors will perform analyses that demonstrate the extremely low frequency of occurrence, or impossibility, of such events for their reactor design, therefore alleviating the vendor from the obligation to perform MST assessments for such reactor transients. It is the responsibility of the vendor to provide the necessary justification for this exclusion (or if the choice is made to include such scenarios, perform the necessary analyses to demonstrate that regulatory criteria are satisfied).

Key Project Point

Phenomena related to extremely unlikely metal fuel SFR transients, such as core disruption (energetics) and loss of primary sodium accidents, were excluded from the trial MST calculation, as it is assumed that SFR vendors will perform analyses justifying the exclusion of such transients from those that require a MST assessment, due to the extremely low frequency, or impossibility, of occurrence.

The proper modeling of benign termination of transient scenarios (*i.e.*, the avoidance of core energetics) is considered here as an accident analysis modeling concern, rather than a source term modeling issue. However, as will be seen in the following subsections, when issues with benign termination modeling were encountered, they were noted to assist in future research and development efforts.

2.2.1 Methodology

The analysis tool chosen for the simulation of the transient scenarios, and the prediction and characterization of core damage, was the U.S. SFR severe accident code SAS4A/SASSYS-1 version 5.1 [7]. Originally developed in the 1960s, SAS4A/SASSYS-1 is now widely used both domestically and internationally for the assessment of SFR transient scenarios. Although SAS4A/SASSYS-1 has not formally been used as part of the U.S. NRC reactor licensing process in the past, there are current Argonne projects investigating the requirements for regulatory acceptability [8].

SAS4A/SASSYS-1 is capable of assessing reactor system conditions, such as primary and intermediate circuit temperatures and pressures, as well as determining detailed core conditions. SAS4A/SASSYS-1 contains several internal modules, which are used for the prediction of fuel pin failure and relocation of molten fuel. It is important to note that many of these modules were originally developed for oxide fuel as part of the Clinch River Breeder Reactor Project (CRBRP). Following the termination of the CRBRP, many of these modules were updated to include metal fuel phenomena during the Integral Fast Reactor (IFR) project in the 1980s and early 1990s. However, this work ceased with the termination of the IFR project in 1994, and the metal fuel core damage models were not formally completed. This is a known gap regarding the modeling of metal fuel SFR core damage accidents and there are efforts currently underway at Argonne to complete the development of the metal fuel core damage modules, in collaboration with the Korean Atomic Energy Research Institute (KAERI) [9]. While code development work is ongoing, the latest SAS4A/SASSYS-1 core damage models were not yet available for use as part of this project. Therefore, for the current MST trial calculation, what is referred to here as the legacy SAS4A/SASSYS-1 metal fuel core damage models were utilized. As will be described in subsequent sections, the limitations of the legacy SAS4A/SASSYS-1 core models required several modifications and assumptions to the trial MST calculation. Any such actions are noted in their respective sections, with a discussion of possible impacts on the MST trial calculation.

The SAS4A/SASSYS-1 model of the reference reactor contained three channels to model the core, each representing one of the fuel batches shown in Table 2-4. The three-channel design was selected to simplify the analysis and expedite code run-times. SAS4A/SASSYS-1 is capable of more detailed core models, including the use of separate channels for each fuel assembly within the core. These options could be used if a vendor wished to characterize core damage with greater precision than the analysis presented here. For the trial MST calculation, the emphasis was on demonstrating the analysis capabilities. The following two subsections describe the results of the SAS4A/SASSYS-1 simulations for the two transient scenarios.

2.2.2 Protected Loss of Flow with Degraded Decay Heat Removal (PLOF+)

The first transient scenario modeled was a protected loss of flow with severely degraded decay heat removal capabilities, referred to here as a PLOF+³. This scenario could represent a loss of offsite power (assuming no emergency diesel generator or other source of AC power) coupled with degraded emergency decay heat removal. Such an event could be caused by extreme weather conditions, such as a very severe

³ The plus sign has been added to the transient name to indicate that the transient is more severe than the historical PLOF definition, which does not include degraded decay heat removal.

winter storm, that disables the electrical grid while also causing snow and ice to accumulate on the DRACS inlets, significantly reducing the DRACS performance for some period of time.

The timeline of the PLOF+ transient is shown in Table 2-7. The scenario begins with the loss of primary flow and heat removal through the intermediate loop and balance of plant. All pumps are assumed to coastdown successfully. Soon after this event, the reactor protection system causes a reactor SCRAM due to a reduction in primary pump discharge pressure. The DRACS system is assumed to be degraded from time zero, with restoration occurring after three days (72 hours). The analysis time is seven days following the initiation of the transient. This time period was chosen based on simulations, which showed that primary system temperatures return to near-nominal conditions at this time.

Table 2-7: PLOF+: Transient Timeline

Time	Event	Description
0 sec	Loss of Primary Flow	Loss of primary pumps with successful coastdown
0 sec	Loss of Balance of Plant Heat Removal	Secondary side trip
0 sec	Degraded DRACS	DRACS operating at <1% of design capacity
2 sec	Reactor SCRAM	Reactor SCRAM on low primary pump discharge pressure
72 hrs	Decay Heat Removal Restored	Decay heat removal restored at 100% of design capacity
168 hrs	End of Analysis	End of analysis as primary system temperatures reach near-nominal temperatures

The PLOF+ scenario was modeled using SAS4A/SASSYS-1 and the input described in Section 2.2.1. The results of this simulation can be seen in Figure 2-5, which includes a ten hour steady-state period at the start of the simulation. Following the initiation of the transient, core and primary system temperatures initially drop, as reactor shutdown occurs. However, absent a heat removal pathway, core and primary system temperatures soon begin to increase. By three days, fuel pin cladding temperatures are around 875°C, with hot pool temperatures approaching 850°C. The slight difference between the hot pool and cold pool temperatures is a consequence of the small amount of residual heat removal through the degraded DRACS. Temperatures begin to fall following the initiation of decay heat removal after three days. By seven days, core and primary system temperatures are near nominal temperatures at 100% power.

As Figure 2-5 shows, fuel pin failure occurs at different times for the three fuel batches, even though they are all at approximately the same temperature. The unique fuel batch pin failure times are largely a result of the different internal fuel pin pressures. Channel C is the first fuel batch to experience pin failure, as it represents the highest pressure fuel pins (at ~10% burnup). This is followed by the failure of fuel pins in Channel B, and finally fuel pin failure of the lowest burnup fuel in Channel A. The properties of each fuel batch at the time of failure are shown in Table 2-8. For the analysis conducted here, it is assumed that all fuel pins within the fuel batch (60 assemblies × 271 pins = 16,260 pins per fuel batch) fail at the same time. This is a simplifying assumption, as the assemblies, and pins within the assemblies, will experience different coolant conditions and have slightly different internal pressures. As stated at the beginning of this section, it is possible to increase the number of channels in SAS4A/SASSYS-1 for greater precision, but that was not the focus of the current analysis.

Figure 2-5: PLOF+: Primary System and Peak Cladding Temperatures⁴

Table 2-8: PLOF+: Fuel Failure Details from SAS4A/SASSYS-1

Characteristic	Ch A	Ch B	Ch C
Time of Failure (hr) ¹	31.89	28.98	22.65
Fuel Temp at Failure (°C)	754	741	719
Hot Pool Temp at Failure (°C)	661	641	612
Internal Pin Pressure Immediately Prior to Failure (MPa/psi)	0.64/92	3.85/558	8.69/1260
Number of Fuel Pins Assumed to Fail	16,260	16,260	16,260

¹From initiation of transient

The legacy SAS4A/SASSYS-1 internal modules for the modeling of fuel pin failure appear to produce a reasonable result, when compared to past testing⁵. This is not surprising, as the SAS4A/SASSYS-1 internal module for the prediction of fuel failure without fuel melting (module DEFORM-5) utilizes correlations based on experimental testing [7, 10]. For example, past tests have shown a cladding penetration rate of approximately 0.005 to 0.01 μm per second for U-Pu-Zr fuel with HT-9 cladding in the 700 to 750°C temperature range [11]. The reference reactor fuel has a cladding thickness of 560 μm . This translates to complete cladding penetration in 56,000 to 112,000 seconds (15 to 31 hours). However, complete cladding penetration is not needed for fuel pin failure to occur for fuel batches B and C, as they are at high internal pin pressures. Therefore, fuel pin failure can occur sooner, which aligns with the results from SAS4A/SASSYS-1. Fuel Batch A, which is at relatively low internal pin pressure, experiences fuel pin failure only after subjected to temperatures over 700°C for over 13 hours.

⁴ Plot includes 10-hour steady-state before transient initiation, to illustrate nominal reactor conditions.

⁵ The predicted pin failure times are likely slightly conservative. Due to the lack of detailed design information, several conservative assumptions were used as part of the SAS4A/SASSYS-1 input concerning fuel pin failure prediction. However, these factors have essentially no impact on the remainder of the MST trial calculation.

2.2.3 Severe Unprotected Transient Overpower (UTOP+)

The second transient scenario modeled was a severe unprotected transient overpower, referred to here as UTOP+⁶. As discussed at the beginning of this section, this scenario was selected to represent the class of SFR transients that may involve fuel melting, and the particular UTOP+ scenario chosen here is likely a very low frequency event, and depending on the reactor design, may not need a detailed MST analysis. However, as explained later in this subsection, such a severe UTOP+ scenario was selected due to several modeling and data constraints.

As discussed in Section 2.2.1, the metal fuel damage models of SAS4A/SASSYS-1 were not formally completed before the termination of the IFR project. While SAS4A/SASSYS-1 was able to successfully complete the analysis of the PLOF+ scenario, the modeling of the UTOP+ scenario was more challenging due to the extent of fuel melting and relocation. The UTOP+ scenario involved SAS4A/SASSYS-1 internal modules that were not needed in the PLOF+ analysis. These modules, although capable of successful execution as part of SAS4A/SASSYS-1 simulation, can be difficult to utilize due to incomplete development efforts. Therefore, for the UTOP+ analysis conducted here, the simulation insights from SAS4A/SASSYS-1 were coupled with experimental results from the metal fuel transient overpower tests conducted at the TREAT facility in the mid-to-late 1980s.

To permit the use of TREAT results within the analysis, a UTOP+ scenario was created that resulted in similar fuel conditions as those seen in the M-Series TREAT tests. The TREAT M-Series tests were a set of very severe transient overpower experiments, conducted on different types of metal fuel. For the analysis here, the most relevant tests are M6 and M7, which contained U-19Pu-10Zr metal fuel at different burnup levels. The results of these tests are provided in Table 2-9. As the table shows, three burnup levels were tested, which coincide very closely with the three fuel batches of the reference SFR design. The three fuel pins were subjected to extreme transient overpowers, reaching over four times nominal power within approximately 10 seconds.

Table 2-9: UTOP+: TREAT Results [12, 13]

Test	Fuel	Burnup (at%)	Peak Overpower (Normalized)	Peak Pressure (MPa/psi)	Fuel Molten[†] (%)	Result
M6	U-19Pu-10Zr	1.9	4.4	3/435	~33.2	No Pin Failure
M6	U-19Pu-10Zr	5.3	4.4	10/1450	~20.6	Pin Failure
M7	U-19Pu-10Zr	9.8	4.0	19/2755	~16.0	Pin Failure

[†]Based on measurements and calculations of liquidus quantity.

Per Table 2-9, the fuel pin at the lowest burnup level (1.9%) was able to withstand the transient overpower without fuel pin failure (although internal fuel melting did occur). Although the two fuel pins at higher burnup levels experienced less fuel melting than the pin at lower burnup, the higher internal pin pressures caused both to experience cladding failure between 9.5 and 11 seconds after the initiation of the transient.

A UTOP+ scenario was created, using the reference reactor design, that resulted in fuel conditions similar to those experienced during the TREAT M-Series tests. Since very high power levels were reached over short time periods in the TREAT tests, the UTOP+ scenario had to be extremely severe. Fuel conditions of the TREAT test could only be matched using a \$0.075 per second reactivity insertion, coupled with reduced radial inherent reactivity feedback. As stated at the beginning of this section, this is an extremely unlikely transient scenario, whose purpose is to create certain core conditions for the subsequent MST

⁶ The plus sign has been added to the transient name to indicate that the transient is more severe than the historical UTOP definition, which is typically of smaller magnitude and without degraded radial feedback.

analysis. The inclusion of the specific UTOP+ scenario in the current analysis should not be misconstrued as an indication of its importance to the future licensing of SFR.

The UTOP+ transient event timeline is provided in Table 2-10. The transient begins with the initiation of the reactivity insertion. The reactor protection system is assumed to fail despite the high neutron flux readings. The SAS4A/SASSYS-1 simulation continued until 11.5 seconds, when the extent of molten fuel movement and relocation caused the termination of the simulation.

Table 2-10: UTOP+: Transient Timeline

Time	Event	Description
0 sec	Reactivity Insertion	Reactivity insertion of \$0.075 per second begins
2 sec	Reactor SCRAM Fails	Reactor SCRAM on high neutron flux fails
11.5 sec	End of Analysis	End of SAS4A/SASSYS-1 analysis

Figure 2-6 illustrates the reactor power level during the UTOP+ scenario. As can be seen, reactor power climbs steadily, to almost 400% at approximately nine seconds, before negative reactivity from molten fuel movement within the fuel pins lowers reactor power. However, the external reactivity insertion continues, driving power above 400% before fuel pin failure and molten fuel movement out of the fuel pin and core region causes power to rapidly decrease. The reactor reaches a peak power level of ~450% at 11 seconds before fuel pin failures begin to occur, which is almost identical to the TREAT M-Series failures that occurred between 9.5 and 11 seconds at 400 to 440% power.

Figure 2-7 shows the primary system and fuel temperatures during the UTOP+ transient. Peak fuel temperatures reach over 1400°C in Channel A (which does not fail during the transient, as in the TREAT tests for low burnup fuel), while Channels B and C experience temperatures of approximately 1250 - 1300°C before pin failure occurs. Although very high temperatures are seen in the core, the hot and cold pool experience almost no temperature change over the 11.5 second simulation period.

Unlike the PLOF+ scenario, where it is assumed that all fuel pins within a fuel batch fail when SAS4A/SASSYS-1 predicts fuel pin failure, only a fraction of the fuel pins within Batch B and C are assumed to experience melting and cladding failure. This change in assumptions is based on the accident phenomena. In the PLOF+ sequence, the reactor is shutdown, but sufficient decay heat removal is unavailable. The failure of fuel pins has essentially no effect on the decay heat generation. Therefore, the core continues to increase in temperature and fuel pin failures continue. In the UTOP+ scenario, the reactor is at greater than 100% power. When molten fuel relocates (both inside and outside of the fuel pin) to an area beyond, or on the periphery, of the active core region, negative reactivity is introduced and reactor power decreases. Therefore, it is very unlikely that all 120 assemblies in fuel batches B and C would experience complete failure before sufficient negative reactivity was introduced to end the transient scenario⁷. Based on this fact, it was assumed that the equivalent of five complete assemblies (5 assemblies $\times$ 271 pins = 1,355 pins) experienced fuel melting and failure in both fuel batch B and C. The fuel pin failure information is summarized in Table 2-11.

⁷ For such an accident sequence, it is also important to consider the possible insertion of positive reactivity following fuel pin failure and the temporary voiding of the coolant channel due to the blow down of the fuel pin.

Figure 2-6: UTOP+: Reactor Power

Figure 2-7: UTOP+: Primary System, Fuel, and Cladding Temperatures

Table 2-11: UTOP+: Fuel Failure Details

Characteristic	Ch A	Ch B	Ch C
Time of Failure (sec)	No Failure	~11	~11
Fuel Temp at Failure (°C)	-	~1300	~1300
Hot Pool Temp at Failure (°C)	-	515	515
Internal Pin Pressure Prior to Failure (MPa/psi)	-	10/1450	19/2755
Number of Fuel Pins Assumed to Fail	-	1,355	1,355

2.2.4 Summary

In general, the transient scenario modeling assessed four phenomena categories, as shown in Table 2-12. Several of these phenomena are central to accurate transient analysis modeling, but are only tangentially important to the source term calculation. The first phenomenon is the benign termination of accident sequences, meaning the avoidance of recriticality or energetics. As stated previously, SAS4A/SASSYS-1 core damage models were not able to complete the UTOP+ transient analysis, but the scenario was purposefully designed in such a way to utilize the results of the TREAT experiments to resolve gaps. This gap in modeling is also currently being addressed through code development work at Argonne.

The second phenomenon was the prediction of fuel pin failure, performed here by SAS4A/SASSYS-1. Again, there are known deficiencies with the SAS4A/SASSYS-1 models, which are currently being addressed, but the code results appeared reasonable (when compared to experimental results) for the PLOF+ scenario. Next was the phenomena related to molten fuel relocation in the UTOP+ transient. This gap did not become a major factor in the source term calculation performed here, as radionuclide release is based on the percentage of molten fuel, not relocation within the fuel channel (as will be described in Section 2.4). Lastly, the modeling of primary system conditions, such as temperature and pressure, was also performed by SAS4A/SASSYS-1, and is not considered a modeling gap, as SAS4A/SASSYS-1 is used internationally for the prediction of primary system conditions during SFR transient scenarios.

Table 2-12: Phenomena Overview – Transient Scenario Modeling

Phenomena	Modeling	Gap?	Impact on MST Trial
<i>Benign termination of accident sequence</i>	SAS4A/SASSYS-1	Partial – “Legacy” core damage modules in SAS4A/SASSYS-1 were unable to model the complete UTOP+ transient, but this gap is known and currently being addressed.	No effect – UTOP+ scenario was designed to utilize TREAT experiment results to resolve gap.
<i>Prediction of fuel pin failure</i>	SAS4A/SASSYS-1	Partial – “Legacy” fuel failure modules in SAS4A/SASSYS-1 predicted pin failure with reasonable accuracy (when compared to past tests). Current efforts ongoing to update metal fuel failure models.	No effect – UTOP+ scenario was designed to utilize TREAT experiment results to resolve gap. PLOF+ predictions approximately match experimental results.
<i>Molten fuel relocation</i>	SAS4A/SASSYS-1	Partial – “Legacy” core damage modules in SAS4A/SASSYS-1 were unable to model the complete UTOP+ transient, but this gap is known and currently being addressed.	No effect – Molten fuel relocation is not a factor in the MST calculation, as radionuclide release fractions are based on molten fuel fraction (which utilized TREAT experiment results for UTOP+). Further discussion in Section 2.4.
<i>Primary system conditions (temperature, pressure, etc.)</i>	SAS4A/SASSYS-1	No	N/A

2.3 In-pin Radionuclide Distribution

As with any nuclear fuel, during the irradiation of sodium-bonded metal fuel, fission products are formed. The characteristics and distribution of fission products within the fuel pin during irradiation is an important factor in determining the extent of radionuclide release after cladding failure. This section assesses the distribution of radionuclides within the fuel pins of the reference reactor, prior to the transient scenario and fuel pin failure.

2.3.1 Methodology

This analysis step can be split into two stages. First, the radionuclides within the fuel pin at the time of the transient must be determined. This is followed by an assessment of the distribution of the radionuclides within the fuel pin at the time of transient. The first step is straightforward, requiring only details about the reactor fuel type, burnup conditions, etc., and an isotope generation and depletion code, such as ORIGEN [14], which was used here. The second part of the analysis, concerning radionuclide distribution within the fuel pin, is more complex.

Before noting the methodology used to develop radionuclide migration fractions for the reference reactor, it is important to describe the phenomena that occur within metal fuel pins during irradiation. As shown in Figure 2-8, before irradiation, the fresh fuel matrix is surrounded by bond sodium. By approximately one percent burnup, the creation of fission products, particularly fission gases, within the fuel matrix causes the fuel matrix to expand (both radially and axially), coming in contact with the cladding and extruding much of the bond sodium to the upper fission gas plenum. Once the burnup exceeds approximately two percent, the porosity of the fuel matrix, formed by the creation of fission products, begins to interconnect. The interconnected porosity provides a pathway for gaseous fission products to migrate to the fission gas plenum. However, non-gaseous radionuclides also migrate within the fuel matrix and to the bond sodium. The interconnected porosity of the fuel matrix also allows bond sodium to become “logged” within the fuel matrix.

Determining the behavior of radionuclides within the fuel pin during irradiation is a difficult process. For comparison, in the development of source term models for LWR fuels, very simple models, such as the Booth model [15], were used to describe radionuclide migration and release from fuel, where the parameters of the model were tailored to reproduce experimental results. The formation of interconnected porosity in metal fuel provides not only an opportunity for migration of radionuclides from the fuel matrix but also for radionuclides to react and form chemical compounds that could affect their migration. Although important insights could be gained from a first principles approach to modeling these reactions and the processes affecting migration, in this analysis an empirical approach is used.

Most data regarding radionuclide migration come from post-irradiation examinations (PIEs) of irradiated metal fuel pins. As part of a recent study of radionuclide release from failed metal fuel pins (ANL-ART-38 [6]), Argonne analyzed PIEs of irradiated metal fuel pins. The PIE data were coupled with information from past fuel pin failures to develop estimates of radionuclide migration within the fuel pin. This report formed the basis of the radionuclide migration fraction estimates described in the following subsection.

Figure 2-8: Formation and Migration of Radionuclides in Metal Fuel

The reference reactor contains three fuel batches, each at different burnup levels. It is assumed that the fuel within each fuel batch is at approximately the same burnup level and that radionuclide migration within the fuel pins of each batch is also approximately the same. For some radionuclides, such as the noble gases, there is considerable PIE available regarding their migration within the fuel pin during irradiation, and the uncertainty associated with their behavior is small. However, for other elements, there is significantly less data available (a gap noted in ANL-ART-38). When data were lacking or uncertainty was large, conservative estimates were made regarding radionuclide migration from the fuel matrix. In this case, conservative means that migration from the fuel matrix to the bond sodium or plenum region was assumed to be on the high-side of available data. Based on the methodology from ANL-ART-38, a minimum migration fraction of 0.1% of the pin inventory was used.

2.3.2 Results

Since this analysis step assesses fuel pin conditions prior to the initiation of the transient, the results are the same for both the PLOF+ and UTOP+ scenarios. The radionuclide inventory calculation was completed first, utilizing ORIGEN to determine the inventory in each of the three fuel batches for the reference reactor fuel type and irradiation conditions. The results of this calculation are provided in Appendix A.1 for the isotopes considered for source term analyses, which are provided in Table 2-13. The table includes

those elements noted in NUREG-1465 [16], and also uranium. In total, over 750 isotopes were recorded and assessed for the MST calculation⁸.

Table 2-13: Elements Considered for Source Term Analysis

Group	Elements
<i>Noble Gases</i>	<i>Kr, Xe</i>
<i>Halogens</i>	<i>I, Br</i>
<i>Alkali Metals</i>	<i>Cs, Rb</i>
<i>Tellurium Group</i>	<i>Te, Sb, Se</i>
<i>Barium, Strontium</i>	<i>Ba, Sr</i>
<i>Noble Metals</i>	<i>Ru, Rh, Pd, Mo, Tc, Co</i>
<i>Lanthanides</i>	<i>La, Zr, Nd, Eu, Nb, Pm, Pr, Sm, Y, Cm, Am</i>
<i>Cerium Group</i>	<i>Ce, Pu, Np, U</i>

The analysis of radionuclide migration within the fuel pin was completed next, using insights from ANL-ART-38. The results of the analysis can be found in Table 2-14. The migration estimates shown are for metal fuel at the burnup levels of the three fuel batches (~2%, 5%, and 10%). As the results show, the fraction of the noble gases present in the plenum increases significantly between 2% and 5% burnup, but begins to level-off as burnup approaches 10%. The available data suggest the iodine migration to the bond sodium is fairly burnup independent. Cesium is one of the most mobile radionuclides, with approximately half of the cesium inventory in the bond sodium by 10% burnup. New data suggest strontium migration may be larger than previously thought⁹. The noble metals and lanthanides experience relatively little migration, with the exception of europium, which appears to exhibit behavior similar to that of cesium. Past tests have observed very small fractions of plutonium dissolved in the bond sodium during prolonged irradiation [18]. Therefore, the minimum migration fraction of 0.1% of the inventory was used.

Table 2-14: In-Pin Radionuclide Distribution Estimates¹⁰

Element	Percentage of Radionuclide in Plenum Region (including bond sodium)		
	Batch A (~2% BU)	Batch B (~5% BU)	Batch C (~10% BU)
<i>Kr, Xe</i>	30.0%	70.0%	75.0%
<i>I, Br</i>	10.0%	10.0%	10.0%
<i>Cs, Rb</i>	15.0%	40.0%	50.0%
<i>Te, Sb, Se</i>	1.0%	1.0%	1.0%
<i>Ba</i>	5.0%	10.0%	15.0%
<i>Sr</i>	5.0%	25.0%	50.0%
<i>Ru, Rh, Pd, Mo, Tc, Co, La, Zr, Nd</i>	0.1%	0.1%	0.1%
<i>Eu</i>	15.0%	40.0%	50.0%
<i>Nb, Pm, Pr, Sm, Y, Cm, Am</i>	0.1%	0.1%	0.1%
<i>Ce</i>	1.0%	1.0%	1.0%
<i>Np, Pu, U</i>	0.1%	0.1%	0.1%

There was one additional calculation step to the in-pin radionuclide migration analysis that was specific to the PLOF+ transient scenario. As shown in Section 2.2.2, in the PLOF+ transient, fuel pin failure occurred

⁸ It is important to also include stable isotopes, as they can affect the formation of compounds, the gas-to-liquid ratio in the fuel pin plenum, and bubble formation behavior in the coolant channel post-fuel pin failure.

⁹ The findings of ANL-ART-38 indicated that less than 1% of the strontium inventory was likely to migrate to the bond sodium during irradiation. However, recent, more detailed PIE data from the METAPHIX tests in Japan indicate that strontium migration may be much higher (with as much as 50% of the strontium inventory in the bond sodium by 10% burnup) [17]. This larger percentage was used for the analysis presented here, to examine the impact of such a release.

¹⁰ Based on the ANL-ART-38 analysis methodology, a minimum migration fraction of 0.1% was used.

anywhere from 22 to 32 hours after the initiation of the transient. Since the PLOF+ is a protected transient, with reactor shutdown occurring within seconds of the transient initiation, radioactive decay changes the radionuclide inventory within the fuel pins by the time fuel pin failure occurs.

While calculating the decay of radionuclides and their daughter products is straightforward, the decay analysis becomes difficult due to the location of the parent/daughter within the fuel pin. For example, some isotopes of krypton within the fission gas plenum will decay into rubidium. The daughter product rubidium will still be present within the fission gas plenum once it is formed (although it may condense or settle onto the bond sodium in the plenum). Therefore, the decay calculation had to account for the location of each parent isotope within the fuel pin.

For each of the three fuel batches, ORIGEN was used to assess the decay of each radionuclide within the fuel pin. Separate ORIGEN calculations were conducted for each region of the fuel pin (plenum/bond sodium and fuel matrix) to ensure that daughter products would be placed at the proper location. Significant effort was involved with properly tracking isotopes within the fuel and ensuring the multiple ORIGEN inputs were correct. The results of these calculations can be found in Appendix A.1. In general, there is a significant reduction in the radionuclide inventory of the fuel pin due to the 22-32 hours of decay.

2.3.3 Summary

Several phenomena were modeled during this analysis step, as shown in Table 2-15. First, the formation of radionuclides during irradiation was determined using ORIGEN. This was followed by an assessment of the migration of radionuclides within the fuel pin during irradiation. There are no computer codes that simulate this process. Instead, the findings from a recent Argonne study (ANL-ART-38) were used as the basis for the migration fraction estimates. These estimates are based on the analysis of past metal fuel PIE data and fuel failure incidents. A partial gap exists due to insufficient data regarding radionuclide migration for several elements important to the source term (such as, I, Te, Ba, Sr, and Eu). Further detail on these gaps is provided in ANL-ART-38 [6]. Due to this uncertainty, what is believed to be, conservative migration fractions were used for several elements. Lastly, for the PLOF+ transient, radionuclide decay within the fuel pin occurs after reactor shutdown, but before fuel pin failure. ORIGEN was utilized to conduct the analysis, but significant analyst effort was also necessary to prepare the multiple ORIGEN inputs that represented different regions of the three fuel batches, which was necessary for proper radionuclide tracking within the fuel pin.

Table 2-15: Phenomena Overview – In-Pin Radionuclide Distribution

Phenomena	Modeling	Gap?	Impact on MST Trial
Radionuclide formation during irradiation.	ORIGEN	No	N/A
Radionuclide migration within the fuel pin during irradiation	No computer code exists. Results based on findings of ANL-ART-38, which examined metal fuel PIE and past fuel pin failure incidents.	Partial – Data regarding the migration of some elements (I, Te, Ba, Sr, and Eu) are sparse. Gap detail provided in ANL-ART-38.	Conservative (Probable) – What is believed to be conservative migration fractions were used for elements where data are lacking.
Radionuclide decay in-pin (for PLOF+ transient)	ORIGEN	No	N/A

2.4 Failed Pin Radionuclide Release

Once the pre-transient in-pin migration of radionuclides has been established, and the transient scenario modeled, the release of radionuclides from the fuel pin to the primary sodium can be addressed. This step requires several modeling approaches and a multitude of individual analyses.

2.4.1 Methodology

As with in-pin radionuclide migration, it is important to review radionuclide release phenomena before describing the methodology to account for the phenomena. Radionuclide release from failed metal fuel pins is quite different for the two transient scenarios examined here. For the case where the fuel pins fail due to extended exposure to elevated temperatures, with no bulk fuel melting, pin failure is predominately caused by eutectic penetration weakening the cladding in conjunction with cladding hoop stress caused by high internal pin pressures. In metal fuel, the highest fuel pin temperatures usually occur at the top of the active fuel column, due to the high thermal conductivity of the metal fuel and coolant. Therefore, cladding degradation in loss-of-heat-removal events is also generally greatest at the top of the fuel pin.

Figure 2-9 graphically depicts the phenomena that occur when a metal fuel pins fails without bulk fuel melting. The failure of the cladding occurs near the top of the active fuel column, near the boundary of the fission gas plenum region (and where extruded bond sodium has collected). The pressure differential between the fuel pin and the coolant channel can be high. Internal pin pressures can be over 7MPa (~1000psi) for high burnup fuel pins. Conversely, the coolant channel may be at approximately 0.3MPa (~45psi) during loss-of-primary-flow events. The pressure differential results in an immediate blowdown of the fuel pin after cladding failure. The high-pressure vapor and gases in the fission gas plenum push the bond sodium (and radionuclides contained within) out of the fuel pin and into the coolant channel. The rapid depressurization temporarily voids the coolant channel and forms a bubble(s) composed of a mix of radionuclide gases, vapors, and aerosols, and also sodium vapor and aerosol. Radionuclides and bond sodium that were in the liquid form within the fuel pin may now vaporize due to the sudden decrease in pressure. In general, little to no fuel from the fuel matrix is lost to the coolant channel, due to the compatibility of the fuel and sodium coolant.

The process is slightly different if bulk fuel melting occurs. For a scenario such as the UTOP+ transient described in previous sections, which has a rapid rise in fuel temperatures, bulk fuel melting occurs prior to cladding failure. As shown in Figure 2-10, a cavity of molten fuel (and fission products) forms within the fuel matrix. Depending on the particular scenario, the molten fuel cavity may reach the cladding causing pin failure, or the molten fuel cavity may extend to the fission gas plenum and result in molten fuel movement into the fission gas plenum region. The latter is assumed to occur for the UTOP+ scenario here (and was observed in the TREAT M-Series tests). The molten fuel is driven into the plenum region due to the expansion of fission gases contained within. The movement of molten fuel into the plenum region results in the introduction of negative reactivity, as fuel leaves the active core region. The molten fuel at the top of the core region may contact the cladding and cause fuel pin failure (as was observed during the TREAT M-Series tests). Although the figure depicts all bond sodium and non-gaseous radionuclides vaporizing due to the elevated temperatures before fuel pin failure (the middle diagram), some may stay in liquid form due to the very high internal pin pressures, then vaporize as pressure decreases following fuel pin failure.

Figure 2-9: Fuel Pin Failure Phenomena – No Melting

Figure 2-10: Fuel Pin Failure Phenomena – With Melting

Once the cladding fails, the depressurization event is similar to what is predicted in pin failure without fuel melting, but with two significant differences. First, the internal pin pressure is likely higher than what is predicted in a non-melting event, due to the elevated temperatures. Second, molten fuel and solid fuel fragments can now be ejected from the fuel pin along with the fission gases and bond sodium. The ejected molten fuel will likely impact adjacent structure and may begin to freeze.

In terms of modeling the radionuclide release associated with fuel pin failure, there are three major questions that need resolved:

- 1) What radionuclides are released from the fuel pin?
- 2) What state are the radionuclides when they are released?
- 3) What radionuclides will be present in the bubble(s) formed in the coolant channel following release?

The first question, regarding which radionuclides are released from the fuel pin, is directly connected to the in-pin radionuclide migration discussed in Section 2.3. As described in that section, there is no computational tool available to assess radionuclide migration within the fuel pin, and the same is true regarding radionuclide release from the fuel pin. SAS4A/SASSYS-1 is capable of tracking fuel and fission gas movement from the fuel pin into the coolant channel, but it does not explicitly track fission products. Therefore, estimates must be developed based on available data and past accidents. A recent Argonne study (ANL-ART-38) performed this analysis, estimating the quantity of radionuclide release for metal fuel pin failures at various temperatures. This information is used as the basis for the radionuclide release estimates provided here.

The second and third questions are linked, and are equally difficult to assess. There is a large pressure change during fuel pin failure. Radionuclides that may have been in the solid or liquid phase before fuel pin failure may suddenly change states. Additionally, the violent blowdown of the fuel pin following failure likely causes the formation of aerosols and may impact the magnitude and rate of radionuclide vaporization. It is also difficult to estimate how many of these products will be present within the bubble formed in the coolant channel or which will be directly transported to the sodium coolant. A methodology was developed to attempt to account for these phenomena, while also providing bounds related to uncertainties.

The analysis of radionuclides release was split into three phases, as provided in Figure 2-11. First, the “pre-failure” assessment uses the commercial thermodynamic equilibrium computational tool HSC Chemistry 8 [19] to calculate the state of the radionuclides that are present within the bond sodium and fission gas plenum¹¹, as shown in the region highlighted in Figure 2-12. HSC determines both the equilibrium chemical and physical state of the radionuclides based on the internal pin pressure and temperature. This calculation provides information regarding the initial conditions within the fuel pin. During the “peri-failure” stage, HSC is again used to determine the state of radionuclides within the fuel pin. However, there are several differences from the previous stage. First, the pin pressure is now at the post-failure pressure, which is likely substantially lower than the pre-failure internal pin pressure. This increases the quantity of radionuclides that are vaporized and in the gas state. Second, additional radionuclides may have been liberated from the fuel matrix due to fuel melting (based on ANL-ART-38 analysis). These radionuclides are also included in the HSC calculation. Although HSC is an equilibrium code, and the “peri-failure” stage occurs quickly and is unlikely to establish thermodynamic equilibrium,

¹¹ A custom HSC thermodynamic database was developed for the elements examined in the MST calculation. More detail on the creation of the database can be found in Appendix C. HSC was chosen in place of other thermodynamic equilibrium codes because it facilitates the creation of custom databases (unlike codes with fixed databases).

the HSC results are considered conservative in terms of the formation of radionuclide gases. This assumption is based on the observation that vaporization requires a change in state that may be kinetically inhibited [20, 21].

Figure 2-11: Procedure for the Analysis of Released Radionuclide Forms

Figure 2-12: Region of HSC Pin Calculations

The final step of the analysis is the “post-failure” assessment. In this step, the goal is to determine what released radionuclides are present within the bubble(s) formed in the coolant channel. As will be discussed in Section 2.5, the initial radionuclide inventory within the bubble is important for determining the fraction of radionuclides transported to the cover gas region by bubble transport (and bypass of retention within the sodium pool). The formation of the bubble represents very complex phenomena, and there is essentially no data available regarding the formation of radionuclide gas/aerosol bubbles within liquid sodium. Therefore, for the analysis here, two cases were considered that represent the extremes of the range of possible outcomes. In the first case, all radionuclides and bond sodium released from the fuel pin are assumed

to be present within the bubble in either the gas/vapor state or as an aerosol. This assumption maximizes the initial radionuclide inventory within the bubble. In the second case, all released radionuclide gases/vapors are assumed to be within the bubble, but only 10% of the non-gaseous radionuclides and bond sodium are assumed to be within the bubble as aerosols. This was considered to be approximately the minimum quantity of non-gaseous radionuclides that could be present within the bubble initially.

Key Project Point

Due to uncertainties regarding the amount of the radionuclides released during fuel pin failure that become entrained in gas/vapor bubbles in the pool, two bounding cases were explored:

- 1)** “All” of the non-gaseous radionuclides and bond sodium within the plenum become entrained in a bubble.
- 2)** “10%” of the non-gaseous radionuclides and bond sodium in the plenum become entrained in a bubble.

2.4.2 PLOF+

The first calculation conducted for the PLOF+ transient was the pre-failure assessment of radionuclide forms within the fuel pin. This calculation is performed primarily for analyst's knowledge, and the results are not directly used in further analysis steps. An HSC calculation was conducted for each of the three fuel batches at temperatures and pressure immediately prior to fuel pin failure (utilizing the decayed pin inventory discussed in Section 2.3.2). Table 2-16 contains a list of these parameters for each fuel batch. These HSC calculations model those radionuclides within the fission gas plenum (and bond sodium in the fission gas plenum) and use the radionuclide inventories described in Table 2-14. A summary of the calculation results can be found Table 2-17, with complete results for all elements and fuel batches in Appendix A.2. As the table shows, the only radionuclides with an appreciable gas fraction in the plenum region are Xe, Kr, Cs, Rb, and I. HSC also reports the speciation of the elements, with a summary of major species provided in Table 2-18.

Table 2-16: PLOF+: Pre-Failure Fuel Pin Conditions

Parameter	Batch A	Batch B	Batch C
Time in Transient (hrs)	31.89	28.98	22.65
Temperature (°C)	754	741	719
Pressure (MPa/psi)	0.64/92	3.85/558	8.69/1260

Table 2-17: PLOF+: Pre-Failure Radionuclide State Summary¹²

Element	Percentage of Pin Inventory in Region								
	Batch A			Batch B			Batch C		
	In Fuel Matrix	In Plenum Liquid/Solid	Gas	In Fuel Matrix	In Plenum Liquid/Solid	Gas	In Fuel Matrix	In Plenum Liquid/Solid	Gas
Kr	70	0	30	30	0	70	25	0	75
Xe	70	0	30	30	0	70	25	0	75
I	90	9.98	0.02	90	9.96	0.04	90	9.96	0.04
Br	90	10	2.39E-04	90	10	3.38E-05	90	10	3.38E-05
Cs	85	14.82	0.18	60	39.79	0.21	50	49.74	0.26
Rb	85	14.93	0.07	60	39.92	0.08	60	39.92	0.08
Te	99	1	7.69E-22	99	1	2.56E-23	99	1	2.56E-23
Sb	99	1	3.83E-10	99	1	1.29E-10	99	1	1.29E-10
Se	99	1	6.39E-26	99	1	1.83E-27	99	1	1.83E-27
Ba	95	5	1.62E-06	90	10	1.23E-06	90	10	1.23E-06
Sr	95	5	5.44E-05	75	25	1.04E-04	75	25	1.04E-04
Ru	99.9	0.1	9.58E-29	99.9	0.1	1.75E-29	99.9	0.1	1.75E-29

Table 2-18: PLOF+: Pre-Failure Plenum Inventory, Major Species Summary¹²

Element	Gas	Liquid
Kr	Kr	-
Xe	Xe	-
I	CsI, NaI, RbI	NaI, RbI, BaI ₂
Br	NaBr, BaBr	NaBr, CsBr, RbBr
Cs	Cs	Cs, CsBr
Rb	Rb, RbNa	Rb, RbI
Te	-	EuTe, Cs ₂ Te
Sb	-	Sb
Se	-	EuSe
Ba	BaBr	Ba, BaI ₂
Sr	Sr	(solid Sr)
Ru	-	(solid Ru)

Unlike the pre-failure calculation, which was conducted primarily to assist the analyst's knowledge of the system behavior, the peri-failure calculation is important for the following radionuclide bubble transport analysis. The HSC calculation of the fuel plenum conditions was repeated, at the failed-pin pressure, shown in Table 2-19. The drastic decrease in pin pressure results in much greater vaporization of

¹² Complete results can be found in Appendix A.2.

radionuclides. As mentioned previously, while it is known that conditions will not reach equilibrium during the fuel pin failure process, the HSC results are seen as bounding regarding the amount of gas/vapor creation. A summary of the calculation results can be found in Table 2-20, which shows much greater vaporization of Cs, Rb, and I than the pre-failure calculation.

Table 2-19: PLOF+: Peri-Failure Fuel Pin Conditions

Parameter	Batch A	Batch B	Batch C
Temperature (°C)	754	741	719
Pressure (MPa/psi)	0.23/33	0.22/32	0.21/30

Table 2-20: PLOF+: Peri-Failure Radionuclide State Summary¹²

Element	Percentage of Pin Inventory in Region								
	Batch A			Batch B			Batch C		
	In Fuel Matrix	In Plenum		In Fuel Matrix	In Plenum		In Fuel Matrix	In Plenum	
		Liquid/Solid	Gas		Liquid/Solid	Gas		Liquid/Solid	Gas
Kr	70	0	30	30	0	70	25	0	75
Xe	70	0	30	30	0	70	25	0	75
I	90	9.94	0.06	90	9.36	0.64	90	9.12	0.88
Br	90	10	7.29E-04	90	10	7.27E-04	90	10	1.08E-04
Cs	85	14.47	0.53	60	36.15	3.85	50	46.59	3.41
Rb	85	14.78	0.22	60	38.39	1.61	50	48.78	1.22
Te	99	1	2.32E-21	99	1	5.11E-22	99	1	4.34E-25
Sb	99	1	1.16E-09	99	1	2.59E-09	99	1	3.52E-11
Se	99	1	1.93E-25	99	1	3.63E-26	99	1	8.66E-30
Ba	95	5	4.91E-06	90	10	2.47E-05	90	10	8.92E-06
Sr	95	5	1.65E-04	75	25	2.09E-03	75	25	5.23E-04
Ru	99.9	0.1	2.90E-28	99.9	0.1	3.52E-28	99.9	0.1	2.68E-31

The determination of radionuclide release fractions from failed fuel pins was primarily based on the findings of ANL-ART-38. The release fractions are provided in Table 2-21, for each fuel pin region. As the table shows, the ANL-ART-38 analysis concluded that for fuel pin failure in this temperature range, radionuclide release would primarily be from the plenum region, with very little additional release from the fuel matrix. The only exceptions to this are the noble gases (Xe, Kr), where it is conservatively assumed that 100% of the noble gas pin inventory will be released, regardless of the burnup level. It is also conservatively assumed that all radionuclide releases occur instantly with failure of the fuel pin¹³. With the release fractions and radionuclide states established, it is now possible to begin the radionuclide bubble transport analysis, described in Section 2.5.

Table 2-21: PLOF+: Radionuclide Release Fractions

Element	Percentage of Total Pin Inventory Released from Fuel Pin								
	Batch A			Batch B			Batch C		
	From Plenum	From Fuel Matrix	Total	From Plenum	From Fuel Matrix	Total	From Plenum	From Fuel Matrix	Total
Kr, Xe	30	70	100	70	30	100	75	25	100
I, Br	10	5	15	10	5	15	10	5	15
Cs, Rb	15	5	20	40	5	45	50	5	55
Te, Sb, Se	1	0	1	1	0	1	1	0	1
Ba	5	0	5	10	0	10	15	0	15
Sr	5	0	5	25	0	25	50	0	50
Ru, Rh, Pd, Mo, Tc, Co, La, Zr, Nd	0.1	0.9	1	0.1	0.9	1	0.1	0.9	1
Eu	15	0	15	40	0	40	50	0	50
Nb, Pm, Pr, Sm, Y, Cm, Am	0.1	0.9	1	0.1	0.9	1	0.1	0.9	1
Ce	1	0	1	1	1.5	2.5	1	4.5	5
Np, Pu, U	0.1	0	0.1	0.1	0	0.1	0.1	0	0.1

¹³ Instant release of radionuclides is considered a conservative assumption, as it may take some radionuclides (especially those still contained within the fuel matrix) some period of time to migrate within the fuel pin and escape through the cladding breach.

2.4.3 UTOP+

The UTOP+ calculation followed a process similar to that of the PLOF+. Only fuel batches B and C are examined here, since fuel batch A is assumed to remain intact during the transient. First, the pre-failure HSC calculation was performed for the temperatures and pressures shown in Table 2-22. As the table shows, the temperatures and pressures of the UTOP+ transient are considerably higher than the PLOF+. A summary of the HSC pre-failure calculation is shown in Table 2-23. Although the internal pin temperatures are high, this factor is offset by the high internal pin pressure, and vaporization rates are fairly similar to the PLOF+ pre-failure calculation. Major species are shown in Table 2-24, and are also very similar to the PLOF+ transient.

Table 2-22: UTOP+: Pre-Failure Fuel Pin Conditions

Parameter	Batch A	Batch B	Batch C
Time in Transient (sec)	-	11	11
Temperature (°C)	-	1300	1229
Pressure (MPa/psi)	-	10.0/1450	19.0/2755

Table 2-23: UTOP+: Pre-Failure Radionuclide State Summary¹⁴

Element	Percentage of Pin Inventory in Region					
	Batch B			Batch C		
	In Fuel		In Plenum	In Fuel		In Plenum
	Matrix	Liquid/Solid	Gas	Matrix	Liquid/Solid	Gas
Kr	30	0	70	25	0	75
Xe	30	0	70	25	0	75
I	90	9.93	0.07	90	9.93	0.07
Br	90	9.99	5.47E-03	90	9.99	5.47E-03
Cs	60	38.68	1.32	50	48.35	1.65
Rb	60	39.21	0.79	60	39.21	0.79
Te	99	1	1.89E-13	99	1	1.89E-13
Sb	99	1	1.10E-06	99	1	1.10E-06
Se	99	1	1.33E-15	99	1	1.33E-15
Ba	90	10.00	3.44E-04	90	10.00	3.44E-04
Sr	75	24.99	0.01	75	24.99	0.01
Ru	99.9	0.	4.05E-18	99.9	0.1	4.05E-18

Table 2-24: UTOP+: Pre-Failure Plenum Inventory, Major Species Summary¹⁴

Element	Gas	Liquid
Kr	Kr	-
Xe	Xe	-
I	CsI, NaI, RbI	NaI, RbI, BaI ₂
Br	NaBr, BaBr	NaBr, CsBr, RbBr
Cs	Cs, CsNa	Cs, CsBr
Rb	Rb, RbNa	Rb, RbI
Te	-	EuTe, Cs ₂ Te
Sb	-	Sb
Se	-	EuSe
Ba	BaBr	Ba, BaI ₂
Sr	Sr	(solid Sr)
Ru	-	(solid Ru)

The peri-failure UTOP+ HSC calculation was conducted at the temperatures and pressures provided in Table 2-25. Since the primary pumps are still operational in the UTOP+ transient scenario, the coolant channel pressure is slightly higher than in the PLOF+ case, but considerably lower than the pre-failure internal pin pressures. A summary of the HSC peri-failure results can be found in Table 2-26. With depressurization, there is significant vaporization of many radionuclides, with very large percentages of Cs, Br, I, Rb, Ba, and Sr converting to the gas state. As will be described in Section 2.5, these fractions will be utilized to determine bubble behavior in the sodium pool.

¹⁴ Complete results can be found in Appendix A.2.

Table 2-25: UTOP+: Peri-Failure Fuel Pin Conditions

<i>Parameter</i>	<i>Batch A</i>	<i>Batch B</i>	<i>Batch C</i>
Temperature (°C)	-	1300	1229
Pressure (MPa/psi)	-	0.27/39	0.27/39

Table 2-26: UTOP+: Peri-Failure Radionuclide State Summary¹⁴

<i>Element</i>	<i>Percentage of Pin Inventory in Region</i>					
	<i>Batch B</i>			<i>Batch C</i>		
	<i>In Fuel</i>		<i>In Plenum</i>	<i>In Fuel</i>		<i>In Plenum</i>
	<i>Matrix</i>	<i>Liquid/Solid</i>	<i>Gas</i>	<i>Matrix</i>	<i>Liquid/Solid</i>	<i>Gas</i>
Kr	30	0	70	25	0	75
Xe	30	0	70	25	0	75
I	90	0.25	9.75	90	0.25	9.75
Br	90	1.32	8.68	90	1.32	8.68
Cs	60	0.14	39.86	50	0.18	49.82
Rb	60	0.24	39.76	60	0.24	39.76
Te	99	1	1.92E-10	99	1	1.92E-10
Sb	99	0.99	0.01	99	0.99	0.01
Se	99	1	1.58E-12	99	1	1.58E-12
Ba	90	7.45	2.55	90	7.45	2.55
Sr	75	4.20	20.80	75	4.20	20.80
Ru	99.9	0.1	3.95E-14	99.9	0.1	3.95E-14

As for radionuclide release fractions for the UTOP+ transient, Table 2-27 contains the results of the calculation (based on ANL-ART-38 analyses), and provides the releases from both regions of the fuel pin. For some radionuclides, such as the noble gases (Xe, Kr), Cs, Rb, and Eu, it was assumed that the remainder of the inventory present in the fuel matrix would volatilize and escape the fuel pin. For the remaining elements, the calculation utilized the percent of the fuel matrix that had become molten during the transient (based on the TREAT experiments results, provided in Table 2-9). The molten fraction was multiplied by the ANL-ART-38 release fraction estimates for molten fuel for that element (or class of elements). As with the PLOF+ analysis, it is conservatively assumed that all radionuclide releases occur instantly with failure of the fuel pin.

Table 2-27: UTOP+: Radionuclide Release Fractions

<i>Element</i>	<i>Percentage of Total Pin Inventory Released from Fuel Pin</i>					
	<i>Batch B</i>			<i>Batch C</i>		
	<i>From Plenum</i>	<i>From Fuel Matrix</i>	<i>Total</i>	<i>From Plenum</i>	<i>From Fuel Matrix</i>	<i>Total</i>
Kr, Xe	70	30	100	75	25	100
I, Br	10	19	29	10	15	25
Cs, Rb	40	60	100	50	50	100
Te, Sb, Se	1	14	15	1	14	15
Ba	10	10	20	15	5	20
Sr	25	10	35	50	15	65
Ru, Rh, Pd, Mo, Tc, Co, La, Zr, Nd	0.1	0.9	1	0.1	0.9	1
Eu	40	60	100	50	50	100
Nb, Pm, Pr, Sm, Y, Cm, Am	0.1	6.9	7	0.1	5.9	6
Ce	1	3	4	1	3	4
Np, Pu, U	0.1	0.9	1	0.1	0.6	0.7

2.4.4 Summary

There were three main classes of phenomena modeled during this phase of the MST trial calculation. First was the partitioning of radionuclides between the gas and liquid/solid phase while in the fuel pin plenum. HSC was used to model this phenomena, which is based on thermodynamic equilibrium. It is possible that other phenomena, such as kinetics, plays a non-trivial role in partitioning between the gas and liquid/solid state, but there are essentially no available data to compare with the HSC results. Also, it is difficult to determine whether the results of the HSC calculation here are conservative or not, as they are inputs into further trial MST calculations steps.

Second, radionuclide release fractions from failed metal fuel pins to the primary sodium were estimated. There is no computational tool capable of performing this task, but ANL-ART-38 developed radionuclide release estimates based on past data. There are partial gaps regarding this phenomenon, as described in greater detail in ANL-ART-38, and it is unclear whether the assumptions used to develop these release fractions are conservative in all cases.

Lastly, the timing of radionuclide release from failed fuel pins (meaning when radionuclides leave the fuel pin, not when the fuel pin fails) was not mechanistically treated, as no computational tool exists. Instead, all radionuclide releases were assumed to occur instantaneously with pin failure. This is a conservative assumption, as there will be a delay as some radionuclides migrate through the fuel pin to the cladding breach site. The instant release assumption maximizes the radionuclide inventory in radionuclide bubbles (maximizing bypass of the sodium pool) and maximizes the inventory within the sodium pool at a given moment, which increases the amount of vaporization to the cover gas region.

Table 2-28: Phenomena Overview – Failed Pin Radionuclide Release

Phenomena	Modeling	Gap?	Impact on MST Trial
Radionuclide partitioning between gas and liquid/solid in plenum region	HSC	Partial – HSC is a thermodynamic equilibrium code, and it is possible that kinetics and other phenomena play a non-negligible role regarding in-pin behavior.	Unclear – Depending on the particular uncertainties, these factors may reduce or increase the potential release of radionuclides from the fuel pin.
Radionuclide release fractions from failed fuel pins	No computational tool exists. Utilized findings of ANL-ART-38.	Partial – While no computational tool exists, an analysis of past data (ANL-ART-38) was able to develop estimates (with noted gaps) of radionuclide release.	Unclear – While ANL-ART-38 attempted to develop conservative release fractions for elements where data was sparse, there is no guarantee that this is the case.
Timing of radionuclide release from failed fuel pins	No computational tool exists. Assumed instant release of radionuclides with pin failure.	Partial – It is unclear the extent to which some radionuclide releases from the failed fuel pin may be delayed.	Conservative – Instant release maximizes radionuclide inventory available for bubble transport and also maximizes inventory in sodium pool available for vaporization.

2.5 Radionuclide Bubble Transport

Following the analyses to determine the fraction of gases/vapors and aerosols that would be entrained in bubbles within the sodium pool (described in Section 2.4), which are released from the fuel pin subsequent to cladding breach, the scrubbing (or removal) of radionuclides from the bubbles during transport from the core region to the surface of the sodium pool was analyzed. This section provides details of the bubble scrubbing calculation, along with a brief description of the computational code utilized to perform the analysis.

2.5.1 Methodology

The transport of radionuclides through the sodium pool within bubbles involves a variety of phenomena, and the analysis of the transport mechanisms requires a variety of inputs from the transient scenario modeling and failed pin radionuclide release steps. Proper treatment of the blowdown process of gases/vapors and aerosols from failed fuel pins and their transport to the sodium pool surface within a bubble is important, as radionuclides may bypass the sodium pool, a major retention mechanism, and be directly released into the cover gas region, where subsequent transport may occur. While it is assumed that no retention of noble gases occurs in the sodium pool, significant retention of other radionuclides is likely. It is therefore imperative to quantify the amount of radionuclide scrubbing (removal) that occurs from bubbles while passing through the sodium pool.

Figure 2-13 graphically depicts the processes that gases/vapors and aerosols undergo subsequent to fuel pin failure. Prior to fuel pin failure, the gases/vapors are assumed to be in the gas plenum of the fuel pin. During the blowdown process these gases/vapors are released from the fuel pin and can push or carry bond sodium, along with radionuclides in the bond sodium, into the coolant channel. Some radionuclide aerosols may be entrained within the bubbles, while others may be directly released into the sodium pool. Some radionuclides within the bubbles may be removed before the bubble reaches the pool surface.

As shown in Table 2-29, there are many mechanisms which may remove aerosols from the bubbles, including: aerosol capture by Brownian diffusion, inertial deposition, and gravitational sedimentation; aerosol removal associated with vapor condensation; and thermophoresis and diffusiophoresis. Any radionuclides that are scrubbed from the bubbles are then deposited in the sodium pool, while the remaining radionuclides within the bubbles are released into the cover gas region once the bubble reaches the sodium pool surface (assuming the bubbles rupture at the surface). The radionuclides in the sodium pool may volatilize and be released to the cover gas region. The radionuclide release due to volatilization is discussed in more detail in Section 2.6.

Figure 2-13: Radionuclide Bubble Transport and Scrubbing

Table 2-29: Aerosol Particle Scrubbing Phenomena

Phenomenon	Description	Considered in IFR Bubble Code Calculation?
Brownian Diffusion	Random movement of an aerosol particle within a fluid	☒
Inertial Deposition	Impaction of an aerosol particle due to its inertia	☒
Gravitational Sedimentation	Settling of an aerosol particle due to gravity	☒
Vapor Condensation (Sodium)	Aerosol particle removed due to condensing sodium vapor	☒
Vapor Condensation (Non-Sodium)	Aerosol particle removed due to condensing vapor (non-sodium)	☐
Thermophoresis	Motion of an aerosol particle due to a temperature gradient	☐
Diffusiophoresis	Motion of an aerosol particle due to a diffusion gradient	☐

To quantify the amount of radionuclide scrubbing that occurs during the travel through the sodium pool, a computational code developed during the IFR project was utilized [22]. This code will be referred to here as the IFR bubble code, as the code was never formally named or released. The IFR bubble code uses classical theories of aerosol scrubbing, which were developed for the case of isolated bubbles rising through water, with modifications to account for phenomena specific to a pool-type SFR. Additional modifications to the classical theories are incorporated to account for difference between a spherical bubble (for which the classical theories were developed) and ellipsoidal bubble, which are more likely to develop in liquid sodium.

As shown in Table 2-29, the IFR bubble code only considers aerosol capture by Brownian diffusion, inertial deposition, gravitational sedimentation, and the effects of sodium vapor condensation. Thermophoresis, diffusiophoresis, and the effects of vapor condensation of elements other than sodium on aerosol scrubbing are not currently considered in the code, however an attempt to model the effects of the

vapor condensation of elements other than sodium was made through insights from additional HSC calculations. It is assumed that aerosol trapping occurs through particle deposition within isolated bubbles ascending through a sodium pool. Thus, detailed hydrodynamic phenomena such as jet (or plume) flow, bubble agglomeration, bubble shattering, bubble swarms, etc. are not addressed. The models in the code assume a bubbly flow regime (*i.e.*, isolated bubbles ascending through a sodium pool with a well-characterized terminal rise velocity), where the initial bubble size is limited by hydrodynamic instability. The output of the code is a decontamination factor (DF) for each of the four scrubbing mechanisms (Brownian diffusion, inertial deposition, gravitational sedimentation, and condensation), through which aerosols are removed from the bubbles. Multiplying these four DFs together provides the overall total DF. The IFR bubble code has only been validated against bubble behavior in water, not liquid sodium.

Table 2-30 provides a list of the required input parameters for the IFR bubble code. The values for sodium pool depth, sodium pool temperature, cover gas pressure, inlet gas temperature, and inlet gas pressure were derived from the results from SAS4A/SASSYS-1 simulations of the two transient scenarios (PLOF+ and UTOP+). The aerosol particle density and diameter were assumed to be constants for the analysis provided described here. The impact of this assumption is discussed in greater detail in the following two subsections. The inlet gas vapor content was determined from the HSC calculations described in Section 2.4.

Table 2-30: Required Input Parameters for the IFR Bubble Code

Parameter	Description
<i>Sodium Pool Depth</i>	<i>Distance from the top of the fuel assemblies to the surface of the sodium pool</i>
<i>Sodium Pool Temperature</i>	<i>Single value for the temperature of the hot pool</i>
<i>Cover Gas Pressure</i>	<i>Pressure at the sodium pool surface/cover gas region interface</i>
<i>Inlet Gas Temperature</i>	<i>Temperature of the gas at the exit of the top of the fuel assemblies (assumed to be equal to the temperature of the gas in the fission gas plenum of the fuel pin)</i>
<i>Inlet Gas Pressure</i>	<i>Pressure at the exit of the top of the fuel assemblies</i>
<i>Inlet Bubble Diameter</i>	<i>Expected value assuming that the initial bubble size is limited by hydrodynamic instability</i>
<i>Aerosol Particle Density</i>	<i>The density of the aerosol particle</i>
<i>Aerosol Particle Diameter</i>	<i>The diameter of the aerosol particle</i>
<i>Inlet Gas Vapor Content</i>	<i>Mole fraction of each element in each fuel assembly batch (Xe, Kr, I, Rb, Cs, Te, Na)</i>

2.5.2 PLOF+

In the PLOF+ transient scenario, the results from the SAS4A/SASSYS-1 analysis (discussed in Section 2.2.2) were used to determine the input values for the inlet gas temperature, inlet gas pressure, pool temperature, and pool depth for the IFR bubble code. The results of the HSC calculations described in Section 2.4.2 were used to define the mole fraction of each element listed in Table 2-31. A separate bubble scrubbing analysis was conducted for each of the three fuel batches. The expected bubble diameter for each fuel batch was calculated based on hydrodynamic instability [23]. The density of the aerosol particles was assumed to be equal to that of CsI and the diameter of the aerosol particles were assumed to be 0.1 μm . These assumptions are discussed later in this section. The IFR bubble code results for the three fuel batches are shown in Table 2-32.

Table 2-31: PLOF+: IFR Bubble Code Input Parameters

Parameter	Batch A	Batch B	Batch C
<i>Sodium Pool Depth (m)</i>	6.234	6.207	6.149
<i>Sodium Pool Temperature (°C)</i>	661	641	612
<i>Cover Gas Pressure (Pa)</i>	101,325	101,325	101,325
<i>Inlet Gas Temperature (°C)</i>	754	741	719
<i>Inlet Gas Pressure (Pa)</i>	213,102	213,031	212,910
<i>Inlet Bubble Diameter (cm)</i>	2.33	2.34	2.36
<i>Aerosol Particle Density (kg/m³)</i>	4,510	4,510	4,510
<i>Aerosol Particle Diameter (μm)</i>	0.1	0.1	0.1
<i>Inlet Gas Vapor Content (mole %)</i>			
<i>Xenon</i>	83.39	80.46	87.30
<i>Krypton</i>	3.47	5.31	6.05
<i>Iodine</i>	0.01	0.04	0.05
<i>Rubidium</i>	0.02	0.07	0.06
<i>Cesium</i>	0.72	3.40	3.19
<i>Tellurium</i>	0.00	0.00	0.00
<i>Sodium</i>	12.39	10.72	3.35

Table 2-32: PLOF+: Decontamination Factor Results from the IFR Bubble Code

Parameter	Batch A	Batch B	Batch C
<i>Brownian Diffusion DF</i>	2.7864	2.6374	2.4787
<i>Inertial Deposition DF</i>	1.1325	1.1227	1.1175
<i>Gravitational Sedimentation DF</i>	1.0169	1.0157	1.0153
<i>Condensation DF</i>	1.1317	1.1132	1.0303
Overall Total DF	3.6310	3.3478	2.8972

The overall DFs for the PLOF+ transient are relatively small due to several factors. First, the pool temperatures at the time of fuel pin failure are not significantly lower than the inlet gas temperatures. Therefore, very little sodium condensation occurs (which is evident in the condensation DF being approximately unity). The assumed small aerosol diameter (0.1 μm) results in both the inertial deposition DF and the gravitational DF being approximately unity. No data was available to approximate the diameter of the aerosol particles, which has a significant impact of the overall DF. Also, a single aerosol particle density was assumed (4,510 kg/m³) instead of performing a calculation for each major species in Table 2-18. Instead, a sensitivity study was performed to demonstrate the effects of aerosol diameter and density on the total DF.

The results of the sensitivity study are provided in Figure 2-14 for fuel batch C. It is important to note that the total DF is not dependent on aerosol particle densities for values less than approximately 0.03 μm¹⁵. In this region, Brownian diffusion is dominant, whereas inertial deposition and gravitational sedimentation become a greater factor at aerosol particle diameters above 0.03 μm. The results of the sensitivity study demonstrate the importance of aerosol particle diameter and density on the total DF. The values assumed for these parameters in the PLOF+ scenario are in the region where the total DF is near a minimum value. This provides a conservative, but perhaps unrealistic, value for the total DF. However, as no data were available to approximate expected aerosol particle diameters (or densities), conservative values were utilized. It is possible to perform additional IFR bubble code calculations using the densities of the major species identified in Table 2-18, but this calculation was not performed for the current study, as the uncertainty regarding aerosol diameter would still have a significant effect.

¹⁵ This value is specific to the current transient scenario and may differ significantly in other scenarios.

Figure 2-14: PLOF+: Aerosol Diameter and Density Sensitivity Study (Fuel Batch C)

2.5.3 UTOP+

As with the PLOF+ transient, the IFR bubble code inputs for the UTOP+ scenario (provided in Table 2-33) were determined utilizing the SAS4A/SASSYS-1 simulation results in Section 2.2.3 and the HSC calculations in Section 2.4.3. However, aerosol scrubbing calculations were only performed for fuel batches B and C, as fuel pin failure was not predicted in batch A. The same assumed aerosol particle diameter ($0.1\ \mu\text{m}$) and density ($4,510\ \text{kg/m}^3$) were utilized as in the PLOF+ calculation. The results of the IFR bubble code for both fuel batches B and C are provided in Table 2-34.

Table 2-33: UTOP+: IFR Bubble Code Input Parameters

Parameter	Batch B	Batch C
Sodium Pool Depth (m)	6.045	6.045
Sodium Pool Temperature (°C)	515	515
Cover Gas Pressure (Pa)	101,325	101,325
Inlet Gas Temperature (°C)	1,300	1,229
Inlet Gas Pressure (Pa)	253,374	252,893
Inlet Bubble Diameter (cm)	2.40	2.40
Aerosol Particle Density (kg/m^3)	4,510	4,510
Aerosol Particle Diameter (μm)	0.1	0.1
Inlet Gas Vapor Content (mole %)		
Xenon	5.79	8.42
Krypton	0.40	0.59
Iodine	0.11	0.14
Rubidium	0.34	0.50
Cesium	4.58	6.83
Tellurium	0.00	0.00
Sodium	88.78	83.52

Table 2-34: UTOP+: Decontamination Factor Results from the IFR Bubble Code

Parameter	Batch B	Batch C
<i>Brownian Diffusion DF</i>	7.7053	5.3386
<i>Inertial Deposition DF</i>	1.1621	1.1382
<i>Gravitational Sedimentation DF</i>	1.0149	1.0137
<i>Condensation DF¹</i>	15.7217	10.6932
Overall Total DF	142.8751	65.8660

¹Includes sodium and cesium vapor condensation

The overall DFs of the UTOP+ scenario are significantly higher than those of the PLOF+ transient. The largest DF for both fuel batches was the condensation DF. In this scenario, the inlet gas temperatures are much higher (1300°C and 1229°C) than the bulk sodium pool temperature (515°C). At these elevated temperatures, a significant fraction of the bond sodium in the pin is gaseous prior to pin failure, and condenses once it is released from the pin into the sodium pool. Because of the large difference in inlet gas temperatures and sodium pool temperatures, an additional HSC calculation was performed to determine the amount of other gaseous species (in addition the sodium vapor) that would condense while the bubble traveled through the sodium pool. These results indicated significant condensation of cesium vapor. This additional condensation is reflected in the condensation DFs provided in Table 2-34.

As with the PLOF+ calculation, the assumed small aerosol diameter (0.1 μm) results in both the inertial deposition DF and the gravitational DF being approximately unity. A sensitivity study was performed with the UTOP+ results (fuel batch B) to demonstrate the effects of aerosol diameter and density on the total DF. The results of the sensitivity study are provided in Figure 2-15 for fuel batch B. The total DF for the UTOP+ scenario is higher than the PLOF+ for all aerosol densities. This is due to the condensation DF, which dominates in this scenario for all aerosol particle diameters and densities (as the condensation DF does not depend on either of these two parameters in the IFR bubble code). It is important to note that the total DF is not dependent on aerosol particle densities for values less than approximately 0.03 μm^{16} for the same reasons stated in the PLOF+ scenario. The results of the sensitivity study for the UTOP+ scenario demonstrate the importance of aerosol particle diameter and density on the total DF.

Figure 2-15: UTOP+: Aerosol Diameter and Density Sensitivity Study (Fuel Batch B)

¹⁶ This value is specific to the current scenario and may differ significantly in other scenarios.

2.5.4 Summary

The assessment of radionuclide transport in, and subsequent removal from, bubbles within the sodium pool includes many different phenomena, as shown in Table 2-35. The first step of the analysis was the determination of what radionuclides to include within the bubbles. As described in Section 2.4, no computational tool currently exists to evaluate this phenomenon, but it is very important to subsequent radionuclide release to the cover gas region. Therefore, two bounding cases (“all” and “10%” in bubble) were assessed to evaluate the impact on the final offsite release.

Next, there are several bubble and aerosol characteristics that impact the magnitude of radionuclide scrubbing that occurs when the bubble passes through the sodium pool. First, the bubble diameter was assumed to be limited by hydrostatic pressure, which is likely a conservative assumption, as smaller bubbles would aid in radionuclide removal. Second, the particle size of the aerosols was assumed to be 0.1 μm , with a density of 4,510 kg/m^3 . As with the bubble diameter, these are likely conservative assumptions, as they result in radionuclide scrubbing levels near the minimum of the possible range (as shown in Figure 2-14 and Figure 2-15). Finally, the actual removal of radionuclides from the bubbles within the sodium pool was modeled using a code developed during the IFR project. The code includes many, but not all, of the relevant phenomena that impact radionuclide removal. Also, the code has not been validated against experimentation with regard to bubble behavior in sodium.

Table 2-35: Phenomena Overview – Radionuclide Bubble Transport

Phenomena	Modeling	Gap?	Impact on MST Trial
Partitioning of released radionuclides into bubbles or sodium pool	HSC and Sensitivity Analysis	Yes – It is not known what radionuclides released from the failed fuel pins will become entrained in bubbles.	As a major source of uncertainty, the MST trial calculation used two bounding cases to quantitatively assess the impact of the phenomena on the MST trial calculation.
Bubble diameter	Not Modeled – Diameter calculated based on hydrostatic instability	Yes – Data on bubble creation in sodium following the blowdown of a metal fuel pin is not available. Without data to estimate the bubble size distribution, it is difficult to know if hydrostatic instability is the appropriate method for estimating the expected bubble diameter.	Conservative (Probable) – The diameter of the bubble has a significant effect on the total decontamination factor. Smaller bubbles would greatly increase the decontamination factor. The hydrostatic instability limit calculation results in larger bubble diameters, which minimizes the decontamination factor.
Aerosol particle size distribution	Not Modeled – Single value assumed	Yes – A computational tool (and sufficient experimental data) does not exist to adequately assess the size of aerosol particles in the bubble.	Conservative (Probable) – The assumption of a single aerosol particle diameter, resulting in the total DF near its minimum value, likely under predicts the amount of aerosol scrubbing that would occur.
Aerosol particle density	Not Modeled – Single value assumed	Partial – The densities of each species of aerosol could be modeled separately. However, this density is expected to change with temperature and pressure, which vary significantly between the fuel pin prior to failure and sodium pool environment.	Conservative (Probable) – The assumption of a single aerosol particle density results in the under-prediction of the total DF for denser particles (U, Am, Pu), many of which are important contributors to offsite dose.
Scrubbing of vapors and aerosols in radionuclide bubble passing through sodium pool (phenomena in Table 2-29)	IFR Bubble Code	Partial – The IFR bubble code has only been validated against water-based experiments, not sodium experiments, and does not include all pertinent removal phenomena.	Unclear – Without sodium experiments for comparison, it is unclear whether the results of the IFR bubble code are conservative or optimistic.

2.6 Sodium Pool Radionuclide Release

This subsection assesses the release of radionuclides from the sodium pool into the cover gas region, including the results of bubble transport analysis, described in the preceding section.

2.6.1 Methodology

The determination of radionuclide release from the sodium pool to the cover gas region is a complex analysis utilizing the results from three previous calculation steps. There are several pathways in which radionuclides can be transported from the sodium pool to the cover gas. First, as described in the previous section, radionuclides can bypass the pool entirely through transport in a gas bubble. Second, radionuclides within the sodium pool may vaporize to the cover gas region. Lastly, radionuclides may be transported due to other phenomena, such as mechanical forces when bubbles burst at the pool surface, or due to liftoff from cover gas circulation. The first method, gas bubble transport, has already been described. This section focuses on the latter transport methods, but the final releases sum amongst all modeled transport mechanisms.

As shown in Table 2-36, there are a variety of phenomena that influence the transport of radionuclides from the sodium pool to the cover gas region. These include several factors that could result in retention of radionuclides within the pool (plate-out, settling), and others that could increase or retard vaporization from the pool (non-homogenous mixing, localized oxidation). The remainder of this subsection describes the computational tool used to assess transport to the cover gas region, including the assumptions used to address the various phenomena.

Table 2-36: Radionuclide Release from Sodium Pool Phenomena

Phenomenon	Description	Considered in HSC Calculation?
Thermodynamic Effects	The influence on vapor pressure due to chemical species	☒
Kinetic Effects	Chemical reaction rates	☐
Mechanical Forces	Transport to the cover gas due to bubble pop, spraying, or liftoff	☐
Plate-out (Adsorption)	Removal of radionuclides in pool due to interaction with structure	☐
Gravitational Settling	Removal of radionuclides in pool due to settling on structures	☐
Non-homogenous Mixing	Localized concentrating of radionuclides in pool	☐
Localized Oxidation	Creation of oxide film on pool surface, slowing vaporization	☐

Radionuclide vaporization from the pool was quantified using fundamental thermodynamic relationships, which were implemented using HSC Chemistry 8. A custom thermodynamic database, compiled for this project, was used to determine the equilibrium distribution of key chemical species (e.g., Cs, I, NaI, CsI) between gas, liquid and solid phases for each step in the transient scenarios. The custom thermodynamic database and the thermodynamic basis for the HSC chemical modeling is presented in Appendix C of this report.

This modeling approach is mechanistic in that it quantifies the thermodynamic driving force responsible for the release of radionuclides from the liquid sodium coolant into the cover gas. Specifically, the model quantifies the equilibrium vapor pressures of radionuclides at a specified pressure, temperature and bulk composition. The vapor pressures are quantified in HSC using a variation of the Redlich-Kwong equation of state and a standard Gibbs free energy minimization algorithm that calls a thermodynamic database populated with species-specific standard values for enthalpy, entropy, and heat capacities [19]. The Gibbs free energy minimization is achieved by a standard Lagrangian-multiplier numerical method. To account for the non-ideality of the fission product/actinide/sodium pool mixture, thermodynamic mixing functions were derived from literature sources and are quantified in the HSC Chemistry model as species-specific

activity coefficients. The derivation of the excess functions and activity coefficients is discussed in Appendix C. Also, an oxygen content of five parts per million was assumed within the sodium pool, which is typically an upper-bound on reactor grade sodium oxygen content [24]. For the PLOF+ and UTOP+ analyses, radionuclides are assumed to remain within the hot pool of the primary sodium circuit, as shown in Figure 2-16. This is considered a conservative assumption, especially for the UTOP+ transient, as primary system flow may disperse radionuclides throughout the system.

Figure 2-16: Region Assessed by HSC for Pool Vaporization

In addition to the thermodynamic mechanism of equilibrium vaporization, kinetic factors may play an important role in the release of radionuclides from the pool to the cover gas. The kinetics of release are influenced by the coolant fluid dynamics, liquid surface area, and other scenario-specific factors. Since many of these kinetic influences are poorly quantified, or are unknown for a particular transient scenario, the chemical model used in this study does not account for specific kinetic processes other than physical bubble transport, as discussed in Section 2.5. The model is therefore likely conservative with respect to kinetic factors in that it is assumed that the radionuclide equilibrium vapor pressures are achieved instantaneously. Specific kinetic and other non-equilibrium processes that could occur at the sodium pool surface, but are not accounted for in the HSC chemical model are:

- Non-homogenous radionuclide mixing in the sodium pool.
- Plate-out (adsorption) and settling of radionuclides within the sodium pool, and condensation or precipitation of volatilized fission products onto cooler steel surfaces of the cover-gas region (the latter is taken into account in the cover gas region analysis in Section 2.7).
- Localized oxidation at the pool liquid/gas interface due to oxygen impurities.
- Spraying due to turbulence (or bubble pop) followed by gas transport by convection.

First, non-homogenous mixing of radionuclides in the sodium pool may occur. This could result in radionuclides concentrating near the cover gas region/sodium pool boundary (or other locations). There is some experimental evidence that indicates cesium and NaI may concentrate near the gas-liquid boundary [25, 26]. However, there is insufficient experimental information to attempt to model this phenomenon. Therefore, perfect mixing within the hot pool is assumed.

Second, plate-out (adsorption) and settling of radionuclides in the sodium pool is not taken into account, although evidence from past accidents and experiments exists indicating that it could occur [5]. However, the available data does not explicitly indicate the temperature or flow conditions at which radionuclide removal would transpire. Condensation or precipitation processes within the cover gas region are not considered here, but these phenomena are discussed in further detail in the cover gas region analysis in Section 2.7.

Localized oxidation at the pool/cover gas interface due to oxygen impurities would tend to slow the volatilization of radionuclides from the pool by forming a thin film of ordered, oxygen bonded species at the pool surface. It is conceivable that some solid radionuclide oxides could be transported, as fine particulate, by gas convection into the cover gas region; however, this process has not been observed experimentally [27, 28].

The spraying phenomenon requires turbulence within the sodium pool and could conceivably be a source of radionuclide bearing-aerosols under highly turbulent conditions, such as boiling, or a bubble swarm reaching the pool surface. The transients assessed in the trial MST calculation do not experience sodium boiling in the primary sodium. Additional releases from gas bubbles popping at the pool surface could occur, but no data was found regarding the possible aerosol formation following this event.

2.6.2 PLOF+

Radionuclide release from the sodium pool to the cover gas region was particularly challenging for the PLOF+ transient scenario. This is due to the extended transient period, multiple fuel pin failure events, and the very high primary system temperatures. Figure 2-17 provides a graphical overview of the analysis procedure. As the figure shows, the transient begins at time zero, with reactor shutdown occurring shortly thereafter. From there, the radionuclide inventory in each fuel pin begins to decay (as was accounted for when determining the inventory in Section 2.3.2). At 22.65 hours into the transient, fuel Batch C fails, releasing radionuclides to the primary sodium. Some radionuclides enter the bubbles, while others directly enter the sodium pool. As the bubbles rise through the sodium pool, bubble scrubbing removes some radionuclides, which then become part of the pool radionuclide inventory. Using this combined inventory (those radionuclides directly released, and those from bubble scrubbing), a vaporization calculation is performed. Those radionuclides that remain in the sodium pool then decay until the next fuel batch failure.

At 28.98 hours into the transient, Batch B fuel pins fail. As with Batch C failure, some radionuclides enter bubbles, while others directly enter the pool, where they join the remains of the Batch C radionuclide release. Following additional bubble scrubbing, another vaporization calculation is performed, followed by the decay of those radionuclides still in the sodium pool. This process is repeated one additional time at 31.89 hours, when fuel Batch A fails.

As described in Section 2.4.1, two different radionuclide bubble cases were considered. In the first case, all radionuclides in the plenum region and bond sodium are assumed to become aerosols within the bubbles. The results of this case are shown in Figure 2-18, for selected elements (complete results can be found in Appendix A.3). In the figure, the radionuclide release to the cover gas is split into six phases, to align with the releases shown in Figure 2-17. As can be seen, vaporization from the sodium pool is essentially negligible when compared to the quantity of radionuclides transported within the bubbles. Only cesium vaporization amounts to greater than one gram of transport. However, due to the large radionuclide inventories in the bubbles (and the very small bubble scrubbing factor, described in Section 2.5.2), very large amounts of cesium are transported to the cover gas region. In addition, heavier elements, such as americium, are also transported to the cover gas region. This is a direct result of the assumptions regarding the amount of these radionuclides in the bond sodium within the plenum prior to fuel pin failure, and the assumption regarding the amount of the bond sodium that becomes entrained within the bubbles following fuel pin failure.

Figure 2-17: PLOF+: Overview of Radionuclide Release to Cover Gas Analysis¹⁷

¹⁷ Bubble transport and vaporization release to the cover gas region are assumed to occur at the same time for each fuel batch, even though there is some separation shown on the figure.

Figure 2-18: PLOF+: Releases to Cover Gas (All in Bubble Case)

Figure 2-19 shows the same results for the “10% in bubble” case. As the figure shows, the release of radionuclides to the cover gas region are essentially reduced by an order of magnitude (other than the noble gases, which are not affected by the 10% assumption). Vaporization from the pool increases slightly, as the inventory in the pool is greater in this case than the “all in bubble” case. However, pool vaporization is still negligible compared to radionuclide transport within the bubbles.

Figure 2-19: PLOF+: Release to Cover Gas (10% in Bubble Case)

One additional HSC pool vaporization calculation was performed to examine the influence of the increase in pool temperatures after the failure of Batch A fuel. As Figure 2-5 showed, Batch A fuel failed when primary sodium temperatures were at 661°C. This is the temperature used for the “Batch A Vap” calculation results presented above. However, the sodium pool continues to increase in temperature, until it achieves a maximum of ~850°C. The higher temperature would likely increase the magnitude of radionuclide vaporization. The HSC calculation performed at 661°C was repeated at 850°C. While an increase in vaporization was seen, the change in the total radionuclide release to the cover gas was

negligible¹⁸. Specifically, the amount of iodine vaporized increased by approximately an order of magnitude, while the amount of cesium vaporized increased by slightly more than double. As Figure 2-18 and Figure 2-19 show, the amount of radionuclide transport from the bubbles still dominates the increased vaporization levels.

2.6.3 UTOP+

The UTOP+ analysis of radionuclide releases to the cover gas region was more straightforward than the PLOF+ scenario. Fuel batches B and C fail at the same time, with no time for radionuclide decay before release. Therefore, bubble transport from fuel batches B and C occurs simultaneously, and only a single vaporization event occurs (as with the PLOF+ scenario, vaporization is assumed to occur instantaneously).

Figure 2-20 provides the cover gas radionuclide release results for the “all in bubble” case, for selected elements (complete results can be found in Appendix A.3). As with the PLOF+ scenario, vaporization from the pool is essentially negligible compared to transport in bubbles. Since far fewer pins fail during the UTOP+ scenario, when compared to the PLOF+ transient, the releases to the cover gas are generally smaller. The lower temperature of the hot pool also aids in bubble scrubbing, reducing releases to the cover gas from bubbles even further. Figure 2-21 has similar results for the “10% in bubble” case. Again, releases are reduced by approximately an order of magnitude, and the increase in vaporization from the pool does not become a major factor.

Figure 2-20: UTOP+: Release to Cover Gas (All in Bubble Case)

¹⁸ Further sensitivity analyses were performed, which indicated that for the pressure conditions assessed (~0.15MPa), sodium temperatures would need to exceed 900°C before vaporization rates of cesium and iodine increased dramatically, and sodium boiling would not occur until approximately 950°C.

Figure 2-21: UTOP+: Release to Cover Gas (10% in Bubble Case)

2.6.4 Summary

The release of radionuclides from the sodium pool to the cover gas region involves many phenomena, as shown in Table 2-37. The first phenomenon (vaporization from the pool, including thermodynamic effects) was directly addressed using HSC. However, the available database is limited, and required significant analyst effort to compile. The specific timing of radionuclide vaporization was not modeled. Instead, a conservative assumption of instant vaporization was used. Several phenomena were ignored, such as kinetic effects, plate-out, and mechanical forces, as no computational tools exist to address these. This results in both conservative and non-conservative impacts. Lastly, perfect mixing was also assumed, which is likely non-conservative, but radionuclides were assumed to remain within the hot pool, which increases vaporization.

Table 2-37: Phenomena Overview – Sodium Pool Radionuclide Release

Phenomena	Modeling	Gap?	Impact on MST Trial
Vaporization from Sodium Pool (Thermodynamic Effects)	HSC	Partial – The modeling tool (HSC) is a well-established, commercial thermodynamic equilibrium solver. However, there are limitations to the available thermodynamic data. While some experimental data exist for quantifying the thermodynamic mixing functions needed to account for non-ideality of the fission product/actinide/sodium pool mixture, there is a need for additional experimental data to properly validate the model. Key species such as NaI, Na and Cs are fairly well understood, but the behavior of other important species such as CsI, and compounds of I, Te, Se, Rb, Br, Eu, and the actinides are less known.	Unclear – The uncertainty in the thermodynamic mixing functions could cause conservative or non-conservative deviations depending on the nature of the molecular interactions described by the mixing functions. Some deviations from ideality can lead to accentuated volatility (i.e., positive deviation from Raoult's Law) and others can lead to attenuated volatility (i.e., negative deviation from Raoult's Law). Experimental investigations are required to resolve this uncertainty.
Timing of Vaporization	Not Modeled – Instant release assumed	Yes – A computational tool (and sufficient experimental data) does not exist to capture time effects of radionuclide vaporization.	Conservative – The assumption of instant vaporization is conservative, as it minimized the time for radioactive decay, and maximized cover gas region inventory.
Kinetic Effects	No Computational Tool Exists – Not modeled	Yes – A computational tool (and associated experimental data) to determine kinetic effects within the sodium pool does not exist.	Conservative (probable) – Kinetic effects would likely decrease the rate of vaporization to the cover gas region, and instant equilibrium vapor pressures are assumed.
Non-homogenous Radionuclide Mixing (Surface-Boundary Concentration)	No Computational Tool Exists – Perfect mixing assumed (in hot pool)	Yes – Although there is some experimental evidence that indicates that non-homogenous radionuclide mixing may occur, the data are insufficient to model the phenomena.	Non-conservative – Non-homogenous mixing could result in radionuclide concentration at the gas/liquid boundary, increasing vaporization.
Plate-out (Adsorption) and Settling in Sodium Pool	No Computational Tool Exists – Not modeled	Yes – Due to a lack of temperature- and flow-dependent information, radionuclide losses in the pool due to adsorption and settling were ignored.	Conservative – Ignoring radionuclide losses in the pool increases the radionuclide inventory available for vaporization.
Mechanical Forces (Liftoff due to Bubble Pop, Turbulence, or Convection)	No Computational Tool Exists – Not modeled	Yes - Due to a lack of data regarding aerosol formation due to turbulence and bubble pop, this phenomenon was ignored.	Non-conservative – Radionuclide releases from the sodium pool to the cover gas would be in addition to the releases from vaporization.

2.7 Cover Gas Region Analysis

The original analysis procedure, as outlined in the project work plan [29], was to utilize a developmental version of CONTAIN-LMR for the assessment of radionuclide transport/retention in the cover gas region and containment. However, due to complications with the implementation of CONTAIN-LMR, detailed results were not available by the end of the current study. The issues encountered with CONTAIN-LMR are discussed further in this section and in Appendix A.4. To allow for the completion of the trial MST calculation within the project timeframe constraints, a simplified radionuclide transport code (referenced here as the SRT code) was developed that utilizes general assumptions to address radionuclide transport phenomena. The following subsection describes the analysis methodology and the capabilities of the SRT code. This is followed by the results of the cover gas region analysis for both the PLOF+ and UTOP+ transient scenarios.

2.7.1 Methodology

The assessment of radionuclide behavior in the cover gas region utilizes the outputs of the bubble transport and sodium pool release analysis steps. Also, outputs from the transient scenario modeling are necessary to establish temperatures and pressures within the cover gas region. Radionuclides that enter the cover gas region may experience a variety of phenomena, as shown in Table 2-38. If there is a reduction in temperatures, radionuclide vapors could condense. Heavier aerosols may settle due to gravitational forces, and smaller aerosols may agglomerate and also settle. Due to the inert (argon) atmosphere of the cover gas region, there are no interactions between the radionuclides and the cover gas, although interactions between the radionuclides themselves and with the sodium vapor are possible.

Radionuclide transport from the cover gas region to containment is most likely a result of leakage from seals around reactor head penetrations. The leakage area is expected to be both temperature- and pressure-dependent, due to the different types of seals used for reactor head penetrations. For example, elastomer seals leak primarily due to permeability, which is temperature dependent, while mechanical seals primary leak due to pressure differentials, such as that between the cover gas region and containment.

Table 2-38: Radionuclide Behavior in Cover Gas Region Phenomena

Phenomenon	Description
Condensation	Reduced temperatures may result in the condensation of radionuclide vapors
Deposition	Radionuclides aerosols may settle on structure or the pool surface due to inertial and gravitational forces. Radionuclide vapors may adsorb (chemisorption and physisorption) on structural surfaces.
Agglomeration	Radionuclide (and sodium) aerosols may agglomerate, changing their properties
Decay	Radionuclide decay will occur
Chemical Interactions	Radionuclides may chemically interact with each other or the sodium vapor
Seal Leakage	Seals in the reactor head will leak depending on temperature and pressure

CONTAIN-LMR

The initial project plan was to utilize a developmental version of CONTAIN-LMR [30] to model radionuclide behavior within the cover gas region (and containment). CONTAIN-LMR is a liquid metal

reactor version of CONTAIN version 1.11 [31], developed in the late 1980s and early 1990s by SNL. However, SNL terminated formal support of the code soon thereafter, and many versions of the code, modified by third parties, now exist. A current project at SNL is transferring the sodium-specific modeling aspects of CONTAIN-LMR into MELCOR [32], which is currently supported by SNL. However, this project was not yet completed at the time of the current work¹⁹, which resulted in the decision to utilize a developmental version of CONTAIN-LMR directly.

As discussed in greater detail in Appendix A.4, several issues soon arose regarding the capabilities of the available version of CONTAIN-LMR, including:

- Inability to model noble gases as gases, rather than aerosols
- Limitation of eight aerosol chemical classes (including a class dedicated to sodium aerosols)
- Limitations in the treatment of pressure-dependent control volume leakage pathways
- Limitations in the treatment of heat structures and heat transfer pathways
- Code instability, resulting in subsequent changes to the source code

Modeling simplifications and gross assumptions were necessary to address these shortcomings within CONTAIN-LMR simulations. Taken together, these modeling choices resulted in unrealistic CONTAIN-LMR results. Although source code modifications were made to address several of these issues, the revised version of CONTAIN-LMR was not available before the completion of the current project. Therefore, the decision was made to use a surrogate, simplified computer code to address radionuclide transport in the cover gas region and containment, in order to allow the completion of the trial MST calculation²⁰.

Key Project Point

Due to complications that arose during the implementation of models in a developmental version of CONTAIN-LMR, and the timeframe constraints of the current project, a surrogate, simplified computer code was utilized to assess radionuclide transport within the cover gas region and containment. Additional detail regarding the issues that were encountered with CONTAIN-LMR is available in Appendix A.4.

Simplified Radionuclide Transport (SRT) Code

Due to the difficulties encountered while implementing models in CONTAIN-LMR, and the condensed timeline of the project, a simplified radionuclide transport code (referenced here as the SRT code for brevity) was developed to allow for analyses of transport/retention phenomena in the cover gas region and containment. The purpose of the code was to allow rapid evaluations of radionuclide transport/retention phenomena, based on simplified assumptions.

The SRT code was developed by Argonne, and is a time-based analysis tool. The SRT code is essentially a zero-D tool that considers three control volumes (the cover gas region, containment, and the environment), with perfect mixing in each volume, as shown in the schematic in Figure 2-22. Flow paths, with user designated leakage rates, are included from the cover gas region to the containment, and from containment to the environment.

¹⁹ The transfer of sodium models into MELCOR is scheduled for completion in 2018. Further information regarding the project can be found in ref [33].

²⁰ Other codes, such as MELCOR could have been utilized in place of the simplified code. However, time constraints of the current project did not permit the development of a new code model.

Figure 2-22: SRT Code Nodalization

Although simple, the SRT code permits an approximation of radionuclide movement from the cover gas region to the containment and environment, while accounting for major impacting factors. The SRT code tracks all (>700) radionuclide isotopes, and assesses radionuclide transport/retention phenomena based on assumptions that the user can modify, such as:

- **Radionuclide Decay and Daughters** – The decay of radionuclides within the cover gas region and containment is included in the calculation, but daughter products are only included for the noble gases.
- **Aerosol Deposition** – Aerosol deposition is assessed using an exponential decay function. All airborne radionuclides (other than the noble gases) are assumed to be in aerosol form, and deposit according to the same decay constant. However, different decay constants can be specified for the cover gas region and containment. No resuspension is assumed.
- **Leakage** – Leakage from the cover gas region into containment, and from containment to the environment, is calculated based on user-specified leakage rates.

Radionuclide decay is included for all isotopes while they are in the cover gas region and containment, with daughter products included for the noble gas isotopes with relatively short half-lives (<5 days). Aerosol deposition is treated through the use of an exponential decay function. All radionuclides, other than the noble gases, are assumed to be in the aerosol form when in the cover gas region or containment (vapors are assumed to either condense to form aerosols or to react and transport with aerosols). A single decay constant is applied to all aerosol radionuclides, although separate decay constants can be used in the cover gas region and containment (a decay constant of $1.1\text{E-}4$ per second was chosen for the cover gas region, and Appendix A.4 has further discussion on the selection of decay constants for the aerosol calculation, which included an assessment of past experiments and analyses). There is no resuspension of aerosols once they have deposited, and no limits are placed on the amount of aerosol deposition that can occur.

Leakage from the cover gas region to containment, and from containment to the environment, is based on a user-specified leakage rate. This is a simplifying assumption, as leakage will likely be both pressure- and temperature-dependent. Since the reference reactor lacks the detailed seal arrangement design necessary to determine actual temperature- and pressure-dependent leak rates, two bounding values were used to assess

this uncertainty. First, a leakage rate of 10.4 cm^3 per second was used, based on information from the Fast Flux Test Facility (FFTF) [34]. This translates into a leakage rate of approximately 0.55 volume percent per day. Second, an upper bound value of 1000 cm^3 per second was used, to simulate a degraded reactor head condition, possible from the failure of a large seal or piping interface. This value translates into a leakage rate of 52 volume percent per day²¹.

Key Project Point

Due to a large uncertainty regarding the design of the reactor head and the magnitude of leakage from the cover gas region into the containment, two bounding cases were explored:

- 1) $10.4 \text{ cm}^3/\text{s}$ (0.55 vol % per day)
- 2) $1000.0 \text{ cm}^3/\text{s}$ (52.0 vol % per day)

As described in preceding sections, both isotopic composition and chemical forms were assessed during the analysis of radionuclide release to the cover gas. However, as shown in Figure 2-23, the SRT code does not take into account chemical species (such as CsI or NaI). Furthermore, as will be discussed in Section 2.9, with the computational tool used for offsite dispersion calculations (WinMACCS), individual isotopes, without regards to their host chemical form, are assessed.

Figure 2-23: Radionuclide Tracking Format for Analysis Steps

Perhaps the biggest shortcoming of the SRT code is the inability to model chemical interactions between sodium vapor/aerosols and oxygen. Since this interaction is of minimal concern for the cover gas analysis, as argon is used within the region, further discussion will be provided in Section 2.8, which details the containment analysis.

For both the PLOF+ and UTOP+ scenarios, the SRT calculation assessed the transport and release of radionuclides over the first seven days (168 hours) of the incident. This extend analysis period requires certain assumptions regarding the transient scenarios and follow-up response. For example, the analysis takes no credit for actions to reduce leakage from the reactor vessel to containment or from the containment to the environment, including efforts to reduce system temperatures or pressures. These are conservative assumptions that result in additional releases to the environment.

2.7.2 PLOF+

Four sets of results are presented for the PLOF+ scenario, as shown in Table 2-39, as both the “all” and “10%” bubble cases (described in Section 2.4) are assessed with both small (0.55 vol%/day) and large (52.0 vol%/day) leakage pathways from the reactor head to the containment.

²¹ Although not considered here due to the limitations of the SRT code, a leakage rate of this magnitude could result in air/water vapor transporting from the containment to the cover gas region and interacting with the sodium pool. Such interactions could cause additional radionuclide vaporization from the sodium pool, increased pool and cover gas temperatures, and an increase in sodium (and sodium oxide) aerosols within the cover gas region.

Table 2-39: Analysis Cases

<i>Case Number</i>	<i>Percentage in Bubble (from Section 2.4)</i>	<i>Reactor Head Leak Rate</i>
1	10%	0.55 vol%/day
2	ALL	0.55 vol%/day
3	10%	52.0 vol%/day
4	ALL	52.0 vol%/day

Detailed results are only presented here for the case numbers 2 and 4, as cases 1 and 3 are very similar, but with non-noble gas inventory reductions of approximately an order of magnitude due to the bubble transport assumptions. Figure 2-24 shows the inventory of selected radionuclides within the cover gas region during the 7-day period. The figure shows the total inventory within the cover gas region, and the quantity removed due to decay, deposition, and leakage for each time step (1 hour). The radionuclides were chosen to illustrate the behavior of different radionuclide groups. Three radionuclide releases to the cover gas occur, at 22.65, 28.98, and 31.89 hours (the radionuclide release due to bubble transport and vaporization at those times is combined to create a single release). The calculation was performed for 168 hours (7 days) following the initial fuel pin failures, for a total analysis time of 191 hours.

As Figure 2-24 illustrates, there is very little radionuclide removal from radioactive decay, as fuel failure begins to occur at over 22 hours after the reactor has shutdown. Therefore, many of the short-lived radionuclides decayed while still within the fuel pin (and their daughter products were accounted for in the analysis conducted in Section 2.3.2). Additionally, no deposition of the noble gases occurs, and their movement to the containment is only a function of the reactor head leakage rate and removal from radioactive decay. For the non-noble gases, aerosol deposition is a major factor, dramatically reducing radionuclide inventories within the cover gas region during the days immediately following fuel pin failure. The reduction in airborne radionuclides due to deposition appears as a straight line on the log plot due to the use of an exponential decay function. In actuality, aerosol removal due to deposition may reach a lower limit, where the concentration of airborne radionuclides is stable, with little additional deposition. However, no lower limit is applied to the calculation results shown here. Due to this assumption, radionuclide transport to the containment for non-noble gases becomes essentially negligible prior to 100 hours after the initiation of the transient.

The fraction of the total core inventory released into containment for all radionuclides of interest is shown in Figure 2-25. The biggest release fractions are for the noble gases, as a large percentage was released from the failed fuel pins, and there is no removal pathway in the sodium pool or cover gas other than radioactive decay. The difference in fuel pin release fractions and radioactive decay accounts for the majority of the difference between the release fractions for the elements in the table.

The results for PLOF+ case 4 are shown in Figure 2-26, where the leakage into containment is two orders of magnitude greater than in case 2. As the figure shows, due to the increased leakage, transport to containment becomes the largest removal mechanism of noble gases in the cover gas region (greater than radioactive decay). However, deposition is still the primary removal pathway for radionuclide aerosols. Complete results are shown in Figure 2-27. As shown in the table, the fraction released into containment is not always directly scalable from case 2, even though the only difference is the leakage rate from the cover gas region into containment. Due to the increased leakage, some radionuclides transport to the containment before they decay in the cover gas region. Therefore, the total transport of radionuclides to containment may be greater than the change in leakage rate between cases 2 and 4 for radionuclides with relative short half-lives. As with case 2, due to aerosol deposition, radionuclide transport to the containment becomes essentially negligible for all radionuclides other than the noble gases within about 100 hours from the onset of the transient.

Figure 2-24: PLOF+ Case 2 - Cover Gas Region Analysis

Figure 2-25: PLOF+ Case 2 - Fractional Release to Containment

Figure 2-26: PLOF+ Case 4 – Cover Gas Region Analysis

Figure 2-27: PLOF+ Case 4 – Fractional Release to Containment

2.7.3 UTOP+

The same cases shown in Table 2-39 were also assessed for the UTOP+ scenario. Figure 2-28 shows the inventory of selected radionuclides within the cover gas region during the 7-day period. All radionuclide releases to the cover gas are assumed to occur at time zero, due to the rapid nature of the transient. Unlike the PLOF+ scenario, radioactive decay is major factor in reducing radionuclide inventories initially, as the fuel pin failures occurred while the reactor was still at power. However, aerosol deposition soon becomes the dominant radionuclide removal pathway several hours after the initial release. By 50 hours after the initiation of the transient, the transport of radionuclides to the containment is essentially negligible for all elements but the noble gases.

The complete list of release fractions to the containment over the 7 day analysis period is shown in Figure 2-29. In general, these fractions are far below those seen in the PLOF+ transient, as far fewer assemblies in the core experienced fuel pin failure. However, the release of krypton and xenon is fairly close to that seen in case 2 of the PLOF+ transient, as the reduced decay time of the UTOP+ transient results in a large inventory of the noble gases, even though far fewer fuel pins failed in the UTOP+ scenario.

Figure 2-30 and Figure 2-31 contain similar results for UTOP+ case 4, where again, the leakage rate to the containment is increased by approximately two orders of magnitude. Here, the impact of reduced decay time of the noble gases results is a release of over 1% of the core inventory of xenon into the containment. For all non-noble gas radionuclides, the releases to containment increase by approximately the same amount as the increase in cover gas leakage rate.

Figure 2-28: UTOP+ Case 2 – Cover Gas Region Analysis

Figure 2-29: UTOP+ Case 2 – Fractional Release to Containment

Figure 2-30: UTOP+ Case 4 - Cover Gas Region Analysis

Figure 2-31: UTOP+ Case 4 - Fractional Release to Containment

2.7.4 Summary

The analysis of radionuclide behavior within the cover gas region is very complex, and involves many phenomena, as shown in Table 2-40. The assessment of modeling gaps is particularly challenging for the cover gas region and containment analyses, as the SRT code was utilized for the analysis described here, but a version of MELCOR with the addition of sodium-specific models will soon be available. Therefore, Table 2-40 discusses the modeling approaches utilized for the current analysis, but also includes capabilities that will be included in the new version of MELCOR when discussing gaps.

SAS4A/SASSYS-1 provides cover gas temperature and pressure. However, SAS4A/SASSYS-1 does not account for heat transfer to the containment or other reactor building structure. The SRT code does not account for these phenomena, since it conservatively uses a constant leakage rate to containment (not temperature- or pressure-dependent). However, such heat transfer capabilities will be available in the new version of MELCOR.

The SRT code accounts for radioactive decay while radionuclides are within the cover gas region and containment, but daughter products are only included for the short-lived noble gases. This is considered a partial gap, as daughter products are typically not included within MELCOR calculations.

There are several phenomena that are not addressed in the SRT code, but that will be modeled in the new version of MELCOR. These include the condensation of sodium vapor, resuspension and re-vaporization, and chemical interactions between radionuclides. The SRT code addresses aerosol deposition through the use of a single exponential decay constant. MELCOR allows class-dependent deposition properties. Neither the SRT code or MELCOR can address aerosol deposition in flow paths, which is likely conservative, as deposition would not only remove airborne aerosols, but also restrict the flow area over time.

Table 2-40: Phenomena Overview – Cover Gas Region Analysis

Phenomena	Modeling	Gap?	Impact on MST Trial
Cover Gas Temperature and Pressure Response	SAS4A/SASSYS-1	No (MELCOR) – Although the SRT code utilized here did not explicitly assess temperature and pressure response in the cover gas region and containment, such capabilities will be available in MELCOR.	Conservative (Probable) – Due to the use of the SRT code, a constant leakage rate (not temperature- or pressure-dependent) was utilized from the cover gas region to the containment.
Radionuclide Decay and Daughter Products	SRT Code	Partial – The SRT Code included radioactive decay for all radionuclides, but included daughter products only for short-lived noble gases.	Non-Conservative – Radionuclide decay is accounted for, which reduces the radionuclide inventory available to transport to the environment. However, the formation of all daughter products is not included.
Condensation of Sodium	Not Modeled	No (MELCOR) – The SRT code did not include the condensation of sodium in the cover gas region. However, MELCOR will include such phenomena.	Conservative – The condensation of sodium would likely increase the removal of airborne radionuclides.
Condensation & Evaporation of Sodium on Aerosols	Not Modeled	No (MELCOR) – The SRT code did not include the condensation/evaporation of sodium on aerosols. However, MELCOR will include such phenomena.	Unclear – This phenomenon will alter the size of aerosols and will impact the degree of deposition.
Aerosol Agglomeration and Deposition	SRT Code	Partial – The SRT code assessed aerosol deposition utilizing a single exponential decay function. MELCOR can address radionuclide class-dependent growth and deposition. Modeling is also dependent on the available data, which is limited.	Unclear – The deposition decay constant utilized in the SRT code is an approximation based on past testing (as described in Appendix A.4).
Resuspension and Re-vaporization	Not Modeled	Yes – Neither the SRT code or MELCOR can model these phenomena. It is unlikely that high flow velocity conditions would arise sufficient to result in resuspension of aerosols. The effect of decay heat on the re-evolution of radionuclides could provide a late release, as indicated in the SOARCA study.	Non-conservative – Resuspension and vaporization would increase the amount of airborne radionuclides.
Aerosol Deposition in Flow Paths	Not modeled	Yes – Neither the SRT code of MELCOR models the deposition of aerosol in flow paths.	Conservative – Radionuclides that would otherwise deposit in a flowpath (such as a leakage pathway from the reactor head) will be available for release to the containment, and the flow path is not reduced due to plugging.
Chemical Interactions	Not modeled	No (MELCOR) – The SRT code did not assess chemical interaction of radionuclide vapors with aerosols. However, to some extent MELCOR will be able to address these interactions.	Unclear – The cumulative impact of chemical interactions on the transport of radionuclides in the cover gas region is unclear.
Seal Leakage	Sensitivity Analysis	Partial – MELCOR is capable of modeling temperature- and pressure-dependent leakage, but sufficient data are needed to estimate leakage functions.	Due to the lack of a detailed reactor design, two values (0.55% vol/day and 52.0% vol/day) were used to assess radionuclide leakage from the cover gas region to containment.

2.8 Containment Region Analysis

The containment region analysis, like the cover gas region analysis, was to originally be assessed using CONTAIN-LMR. However, this part of the analysis was also conducted with the SRT code, due to difficulties encountered with CONTAIN-LMR. The following subsections describe the containment-specific aspects of the modeling methodology, along with the results for the PLOF+ and UTOP+ scenarios.

2.8.1 Methodology

The analysis of radionuclide behavior in the containment requires only the results from the cover gas region analysis²². The radionuclide transport/retention phenomena encountered during this analysis step are almost identical to that of the cover gas region analysis. However, radionuclides entering the containment now have an opportunity to interact with water vapor and oxygen in the air. Also, containment leakage phenomena are different than that of seal leakage from the reactor head.

Table 2-41: Radionuclide Behavior in Containment Phenomena

Phenomenon	Description
Condensation	Reduced temperatures may result in the condensation of radionuclide vapors
Deposition	Radionuclides aerosols may settle on structure or the pool surface due to inertial and gravitational forces. Radionuclide vapors may adsorb on structural surfaces.
Agglomeration	Radionuclide (and sodium) aerosols may agglomerate, changing their properties
Decay	Radionuclide decay will occur
Chemical Interactions	Radionuclides may interact with each other, sodium vapor, and water/oxygen
Containment Leakage	Containment leakage to environment depending on temperature and pressure

- Discussed in Cover Gas Region Analysis section.

As with the analysis of the cover gas region, the SRT code was utilized to assess radionuclide transport and retention within the containment. A single node, with perfect mixing, was used to model the containment atmosphere, which is potentially conservative given the size of the reference reactor containment, as perfect mixing will result in the initiation of leakage to the environment immediately following the introduction of radionuclides to the containment. The most significant drawback of using the SRT code for the assessment of the containment is the lack of chemical interaction modeling in the code, particularly sodium/oxygen reactions, which has several repercussions for the analysis:

- Sodium vapor/aerosol interactions with oxygen in the containment would likely result in the formation of larger sodium oxide aerosols. Airborne radionuclides may deposit on these aerosols, and settle due to gravitational forces. If there is substantial leakage from the cover gas region to the containment, particularly if the leakage path is sufficient for containment air to circulate back through the cover gas region, reaction of sodium vapor or sodium aerosols with air and moisture can produce sodium oxide aerosols, which can grow by agglomeration. Other aerosols produced by

²² If the containment analysis was conducted with a computer code such as CONTAIN-LMR or MELCOR, conditions within the containment (pressure/temperature) would be also be connected to the analysis of the cover gas region and reactor system.

condensation of radionuclide vapors can co-agglomerate with the sodium oxide aerosols. Gravitational settling and the removal of airborne radionuclides can substantially reduce the inventory of radionuclides available to leak to the environment. Multi-aerosol models, like those in MELCOR, are able to consider the effect of mixing of aerosols with different initial size distributions. The use of a single exponential removal constant could either over-estimate or under-estimate this effect depending on the degree of conservatism in the removal constant.

- Sodium vapor/aerosol interactions with oxygen and water vapor are exothermic, and a significant quantity of airborne sodium could result in a appreciable increase in containment temperature and pressure, possibly increasing the leakage rate to the environment. For this analysis, the design basis leakage rate is assumed (1% vol/day) regardless of the temperature and pressure of containment, which is likely conservative for the transient scenarios analyzed.
- Larger sodium oxide aerosols could potentially become trapped in leakage pathways in containment, resulting in leak plugging and reduced radionuclide transport to the environment. This phenomenon is also conservatively ignored.
- Some radionuclide chemical forms may decompose following interactions with oxygen, forming more volatile radionuclide forms. The SRT code does not take into account the chemical form of a radionuclide, and assesses radionuclide removal due to deposition with a single exponential decay constant. This is likely conservative for most airborne radionuclides, but there are likely exceptions.

As described, the sum total of the impact of ignoring chemical interactions with oxygen in the containment is likely conservative, but that is not true for all cases, such as the formation of more volatile radionuclide forms.

As with the analysis of the cover gas region, a single exponential decay constant was utilized to address the deposition of non-noble gas radionuclides. Specifically, a decay constant of $5.5\text{E-}5$ per second was chosen, based on an analysis of past data, described in Appendix A.4.

2.8.2 PLOF+

The containment analysis assessed the four PLOF+ cases outlined in Table 2-39. Detailed results for cases 2 and 4 are presented here. Figure 2-32 shows the time history of several selected radionuclides within the containment. As with the cover gas region analysis, the figure shows the total inventory within the containment, and the quantity removed due to decay, deposition, and leakage for each time step (1 hour). Due to the assumption of perfect mixing in both the cover gas region and containment, radionuclides begin to enter the containment soon after the initial release into the cover gas region. The noble gases, once in containment, are released to the environment according the containment leakage rate, with only radioactive decay reducing the inventory. For non-noble gas radionuclides, deposition is a major removal pathway, resulting in essentially negligible releases to the environment after approximately 100 hours. Figure 2-33 shows the fractional releases to the environment, in terms of total core inventory. By far, the largest fractional release come from the noble gases, as there is no removal mechanism in the containment other than decay.

Figure 2-34 illustrates the fractional releases for all elements considered for the MST analysis over multiple stages of the calculation. This plot is provided to give an indication of where major reductions in the released radionuclide inventory occur. As the figure shows, retention in the fuel pin and sodium pool result in large reductions for the non-noble gases, while additional reductions occur due to deposition in the cover gas region and containment.

Figure 2-35 through Figure 2-37 present similar results for PLOF+ case 4. Here, the large leakage rate from the reactor head results in a much greater radionuclide inventory within containment, which subsequently results in a greater release to the environment.

Figure 2-32: PLOF+ Case 2 - Containment Analysis

Figure 2-33: PLOF+ Case 2 - Fractional Release to Environment

Figure 2-34: PLOF+ Case 2 – Total Percentage Release Results

Figure 2-35: PLOF+ Case 4 - Containment Analysis

Figure 2-36: PLOF+ Case 4 - Fractional Release to Environment

Figure 2-37: PLOF+ Case 4 - Total Percentage Release Results

Lastly, Table 2-42 provides a summary of the cumulative PLOF+ radionuclide release to the environment over the seven day analysis period. As the results show, in terms of activity, the noble gases dominate the release. There is no change in noble gas release between cases 1 and 2, and cases 3 and 4, as the change in assumption regarding radionuclide entrainment within the bubble does not impact the noble gases. However, there is a change in the release of non-noble gases due to the increase in bubble transport. Section 2.9 will discuss the difference between the releases in more detail, including the importance of the modeling assumptions and their impact.

Table 2-42: PLOF+: Total Radionuclide Release to Environment

<i>Case</i>	<i>Activity Release (Ci)</i>		<i>Total</i>
	<i>Noble Gases</i>	<i>Non-Noble Gases</i>	
<i>Case 1</i>	27117	1.15	27118
<i>Case 2</i>	27117	7.95	27125
<i>Case 3</i>	1153300	104.4	1153404
<i>Case 4</i>	1153300	720.6	1154020

2.8.3 UTOP+

Due to the smaller releases associated with the UTOP+ analysis, only detailed results for case 4 are shown here (Figure 2-38 through Figure 2-40), as it is the case with highest release levels. As with the cover gas region analysis, a significant amount of decay occurs within the containment, since the radionuclide release occurred while the reactor was at power. As with the PLOF+ analysis, the release of non-noble gases becomes negligible by 100 hours, while the release of the noble gases obtains a steady state value based on the containment leakage rate and the decay of longer-lived radionuclides.

Complete UTOP+ release results are presented in Table 2-43, which exhibit trends similar to that of the PLOF+ transient. In terms of activity, the noble gases dominate the release, even in the cases with “all” in the bubbles (cases 2 and 4). Section 2.9 will discuss the results in greater detail when reviewing offsite dispersion.

Table 2-43: UTOP+: Total Radionuclide Release to Environment

<i>Case</i>	<i>Activity Release (Ci)</i>		<i>Total</i>
	<i>Noble Gases</i>	<i>Non-Noble Gases</i>	
<i>Case 1</i>	2218	0.01	2218
<i>Case 2</i>	2218	0.03	2218
<i>Case 3</i>	93811	1.00	93812
<i>Case 4</i>	93811	3.05	93814

Figure 2-38: UTOP+ Case 4 – Containment Analysis

Figure 2-39: UTOP+ Case 4 – Fractional Release to Environment

Figure 2-40: UTOP+ Case 4 – Total Fractional Percentage Results

2.8.4 Summary

Although many of the same phenomena experienced during the cover gas region analysis are also applicable to the containment analysis, they are not repeated here. However, there are several phenomena that are unique to the containment analysis, as shown in Table 2-44. The temperature and pressure response of containment was not modeled directly for the analysis here (as leakage rates were temperature- and pressure-independent), but such modeling will be available in a new version of MELCOR. The same is true of chemical interactions with oxygen in the containment, as MELCOR will be able to address this phenomenon directly. Lastly, an assumed value was utilized for containment leakage for the SRT code, but MELCOR will be able to model temperature- and pressure-dependent leakage to the environment.

Table 2-44: Phenomena Overview – Containment Region Analysis

Phenomena	Modeling	Gap?	Impact on MST Trial
Containment Temperature and Pressure Response	Not Modeled	No (MELCOR) – Although the SRT code utilized here did not explicitly assess temperature and pressure response in containment, such capabilities will be available in MELCOR.	Conservative (Probable) – Due to the use of the SRT code, a constant leakage rate (not temperature- or pressure-dependent) was utilized from the containment to the environment.
Chemical Interactions with Water Vapor and Oxygen	Not Modeled	No (MELCOR) – Although the SRT code utilized here did assess chemical interactions with water/oxygen, such capabilities will be available in MELCOR.	Unclear – The cumulative impact of the complete exclusion of sodium/oxygen interactions within the SRT code is unclear.
Containment Leakage	Assumed Value	No (MELCOR) – Although the SRT code utilized a single, constant value for containment leakage, MELCOR is capable of modeling pressure- and temperature-dependent leakage.	Conservative (Probable) – The use of the design basis leakage rate throughout the transient period is likely conservative for both the UTOP+ and PLOF+ scenarios.

2.9 Offsite Dispersion Analysis

The offsite dispersion analysis was conducted utilizing the code WinMACCS. There are many uncertainties related to the offsite dispersion of radionuclides following a core damage transient. The analysis presented in this section is provided as demonstration of the analysis tools for an SFR MST calculation. The resulting dose findings are heavily dependent on the input assumptions and should not be interpreted as an indication of regulatory acceptance.

2.9.1 Methodology

The offsite dispersion analysis requires the output of the containment analysis, plus siting properties. As shown in Table 2-45, there are many phenomena that impact the dispersion of radionuclides offsite. However, most of these phenomena are not unique to SFRs, and are well-characterized from LWR studies. This is not true of all phenomena though, as a metal fuel SFR radionuclide release may have different chemical interactions (and forms) than those radionuclides released following LWR transients, and the applicability of existing dose conversion factors likely requires further assessment.

Table 2-45: Offsite Dispersion Phenomena

Phenomenon	Description	Considered in WinMACCS?
Dispersion	Plume dispersion	☑
Decay	Radionuclide decay	☑
Daughter Products	Daughter products of radioactive decay	☑
Chemical Interactions	The chemical form of the radionuclides and possible interactions	☐
Deposition	Wet/dry deposition	☑
Meteorology	Weather conditions that impact plume dispersion	☑
Siting	Site characteristics	☑
Evacuation	Evacuation of population	☑
Dose Factors	Dose conversion factors for radionuclides	☑

The offsite dispersion analysis was performed using WinMACCS [35], with a calculation of total effective dose equivalent (TEDE) of the maximally exposed offsite individual (MOI) at several distances from the plant. The selection of this criteria was made based on 10CFR50.34 (a)(1) [36], which contains two dose requirements during a fission product release:

- 1) An individual located at any point on the boundary of the exclusion area for any 2-hour period following the onset of the postulated fission product release, would not receive a radiation dose in excess of 25 rem TEDE.
- 2) An individual located at any point on the outer boundary of the low population zone, who is exposed to the radioactive cloud resulting from the postulated fission product release (during the entire period of its passage) would not receive a radiation dose in excess of 25 rem TEDE.

These are not the only regulatory criteria that would be applicable for the licensing of an SFR (see ref [37] for more examples), but they provided a straightforward point of comparison for the offsite dispersion analysis conducted here.

WinMACCS addresses many of the phenomena noted in Table 2-45, and as a popular computational tool for the assessment of offsite dispersion, there are many documents available that describe the models contained within. The focus of the current discussion is the possibility of SFR-specific factors that could impact the offsite dispersion analysis. For example, the radionuclide aerosols released from containment may be of different size and density than those typically released following an LWR transient. However, WinMACCS allows the specification of these parameters, which would accommodate an SFR analysis, if such information was known. Similarly, custom dose conversion factors can be utilized in WinMACCS, as those currently available for the code (such as FGR-13 [38]) may not be directly applicable for the chemical form and species of radionuclide release from an SFR. This possibly discrepancy is not addressed in detail here, as it would likely require significant effort to determine if the chosen dose conversion factor database adequately represents the SFR source term with regard to radionuclide form.

The first step of the offsite dispersion analysis was to down-select from the list of over 700 radionuclides tracked throughout the trial MST analysis. WinMACCS is limited to 150 isotopes per calculation. While separate calculations can be performed and combined to allow for the treatment of more isotopes, an assessment of those isotopes released for the trial MST calculation found only 138 isotopes of importance to offsite dose²³. Table 2-46 contains the major WinMACCS input parameters that were used for the analysis. When possible, conservative assumptions were utilized.

Table 2-46: WinMACCS Input Parameters

Input	Selected Input	Note
Site	Surry	A standard example site
Meteorology	Surry meteorology file	Addressed using stratified sampling
Dose Metric	Centerline dose	MOI metric
Wet Deposition Factor	1.89E-5 1/s, 0.664	From SOARCA analysis [39]
Dry Deposition Velocity	0.01 m/s	NUREG-1150 value [40]
Plume Meander	MNDNOW=NEW	RG 1.145 [41]
Dose Conversion Factors	FGR-13	Ref [38]
Evacuation/Shielding	None	Conservative selection
Release Height	0m	Conservative for locations near plant
Heat	No sensible heat	Reduces plume rise

Seven plume releases was assumed (one for each of the seven days assessed following fuel pin failure), with each plume release lasting one day. The fraction of each radionuclide released during each of the seven plumes was calculated based on the releases from containment for each time period (Section 2.8).

2.9.2 PLOF+

The results of the PLOF+ offsite dispersion analysis can be seen in Figure 2-41, for all four cases from Table 2-39. Distances were selected between 100m and 4,830m (3 miles) from the release site. Both the mean values and 95th percentiles (from the meteorology sampling) are shown. As the figure illustrates, offsite doses are very small, even at distances near the plant, for cases 1 and 2. The difference in assumptions regarding the amount of radionuclides that become entrained in bubbles within the core (the difference between cases 1 and 2), results in approximately an order of magnitude increase in offsite dose. There is a larger increase in dose between cases 1 and 3, than between cases 1 and 2, since the increase in reactor head leakage in case 3 is approximately two orders of magnitude. When accounting for the change in magnitude regarding the assumption, the increases resulting from the change in the bubble entrainment assumption, and the increases due to the assumption regarding reactor head leakage are very similar. This

²³ A complete ranking of isotopes was performed based on the magnitude of the radionuclides released and the applicable dose conversion factors. Those isotopes not selected for inclusion in the WinMACCS calculation had a contribution to dose below 0.1% of the cumulative dose, based on a simplified offsite dose assessment.

indicates that the assumptions associated with bubble entrainment (and transport) can be as impactful on offsite dose as the assumptions related reactor head leakage. The only case that resulted in offsite doses above 25 rem was case 4 (“all” in bubble, and “large” reactor head leakage), but only at a distance of 100m and 200m from the release site.

Figure 2-41: PLOF+: Offsite Dispersion Results²⁴

2.9.3 UTOP+

The offsite dispersion results for the UTOP+ transient are shown in Figure 2-42. In general, the offsite doses are much lower than that of the PLOF+ transient, as far fewer fuel pins failed during the transient, even though the radionuclide release fractions from those pins was high due to the occurrence of fuel melting. The impact of the assumption regarding radionuclide entrainment within bubbles is less than an order of magnitude, and similar to the increase in dose due to the assumption regarding reactor head leakage (when normalized for the magnitude of increase). The resulting dose for all four cases, even at distances very near the release site, are significantly less than 25 rem.

²⁴ Mean value with 95th percentile upper error bar.

Figure 2-42: UTOP+: Offsite Dispersion Results²⁵

2.9.4 Summary

There are many phenomena that can impact the assessment of offsite dose. However, the review here only addresses those phenomena that may be unique to SFR radionuclide releases. Modeling concerns related to general phenomena, such as plume dispersal, meteorology, etc., are well documented elsewhere. For metal fuel, pool-type SFR offsite dispersion analysis, there are three major concerns, as shown in Table 2-47, which all involve the chemical and physical characteristics of the released radionuclides.

The first issue relates to the characteristics of those radionuclides released from the plant, such as aerosol size and density. Due to the presence of sodium vapor/aerosols associated with the release within the containment, aerosol characteristics may deviate from those historically assumed for LWRs. It is likely that the presence of sodium aerosols will result in aerosol agglomeration, but it is difficult to assess the extent to which this factor would distort the applicability of LWR characteristics. Aerosol wet and dry deposition factors from NUREG-1150 and the SOARCA study were chosen, but it is not clear whether these choices are conservative or optimistic for SFR analyses as the particle size distributions are uncertain.

The second issue is the continued possibility of chemical interactions with released radionuclides. If there is a large quantity of sodium released to the containment, it may interact with all available oxygen, limiting further radionuclide-oxygen reactions. Therefore, there is a possibility of continued chemical reactions upon release from containment. As with chemical interactions in the cover gas and containment, it is difficult to determine the cumulative effect of these phenomena, and whether the assumptions utilized here (essentially ignoring this possibility) is conservative in terms of offsite consequence. Unlike the first issue, WinMACCS is not well suited to address the possibility of chemical interactions during radionuclide release.

²⁵ Mean value with 95th percentile upper error bar.

Lastly, the dose conversion factors utilized for the present analysis are based on studies that were focused on LWR radionuclide release. Again, the physical and chemical form of radionuclide release from an SFR could impact the dose conversion factors. However, it may require a substantial effort to assess this phenomenon in detail.

Table 2-47: Phenomena Overview – Offsite Dispersion Analysis

Phenomena	Modeling	Gap?	Impact on MST Trial
Radionuclide Characteristics	WinMACCS	Partial – While WinMACCS allows detailed (and custom) aerosol properties, the applicability of LWR release data for a metal fuel SFR transient is unclear.	Unclear – The impact of deposition factors derived for LWR analyses is not clear.
Chemical Interactions	Not Modeled	Yes – Detailed data regarding the possibility of continued chemical reactions upon release from containment is lacking, and WinMACCS is not well suited for the inclusion of such phenomena.	Unclear – The impact of chemical interactions post-release on offsite consequence is unclear.
Dose Conversion Factors	WinMACCS – FGR-13	Partial – Dose conversion factors exists, but their applicability for the chemical and physical form of radionuclides released during an SFR transient is unclear.	Unclear – The impact of LWR dose conversion factors on offsite consequence is unclear.

3 Sensitivity Calculation

As described in Section 1.2, a sensitivity calculation was performed to provide information regarding the importance of particular radionuclides and transport/retention phenomena to offsite consequence. The results of this study are utilized in Section 4 to prioritize gaps identified during the MST trial calculation. The remainder of this section is organized in the following fashion:

3.1 Study Approach – A description of the study motivation, along with a review of the transients analyzed.

3.2 Source Term Decomposition – A summary of the transport/retention phenomena and how they were modeled for the sensitivity analysis.

3.3 Base Cases – The findings of eight base cases examined using the simplified sensitivity analysis tool.

3.4 Sensitivity Analysis – A description of series of sensitivity cases to explore the importance of different phenomena.

3.5 Findings – A summary of the analysis findings.

Key Project Point

A simplified source term analysis model was developed to explore the importance of specific radionuclides and transport/retention phenomena with regard to offsite consequence.

3.1 Study Approach

Prior to the licensing of an SFR, it will be necessary to develop the technical basis for a MST methodology that would be used in support of a license application. Much of the existing technical basis that has been previously developed has been recently identified in the reports ANL-ART-3 and ANL-ART-38. The magnitude of the research effort undertaken by the U.S. NRC and the nuclear industry in the development of a source term modeling capability for LWRs was very large. The NUREG-1465 report [16] provided the nuclear industry with an Alternative Source Term that was prepared as an alternative to the TID-14844 [42] source term approach, which had been used at the time when most operating plants in the U.S. were first licensed. The NUREG-1465 source terms were based on sensitivity studies performed with the NRC's Source Term Code Package (STCP) [43], which was the predecessor to the MELCOR code [32]. Expert elicitation was used to characterize the range of epistemic uncertainty. Within the U.S., the source term modeling capability has effectively been incorporated into the MELCOR2 (NRC) and MAAP5 (industry) [44] computer codes. The most recent comprehensive examination of LWR source terms was performed by Sandia National Laboratories within the NRC's SOARCA study [45]. A source term analysis capability comparable to the MELCOR code will likely be required for SFRs but with more limited funding than what was available to support LWRs. To help prioritize future additional SFR source term research activities, a sensitivity and uncertainty analysis study has been completed as described in this section.

Although LWRs were designed using the concept of defense-in-depth employing multiple barriers to the release of radionuclides in an accident, early probabilistic risk analyses indicated that in the dominant severe accident scenarios, the primary system boundary was in a failed state at the time of core melting, leaving only the containment system boundary as a barrier to environmental release of radionuclides. In contrast, the SFR designs under development appear to have more robust defense-in-depth features that would reduce the potential for release of radionuclides. For this reason, the approach being taken in this

sensitivity study focuses on the behavior of these barriers. Because of the serial nature of the barriers, their effectiveness in limiting offsite dose can be represented by multiplicative dose-reduction factors. In logarithmic space these factors are additive constants that provide a convenient means of visually displaying how they impact offsite dose.

3.1.1 Transient Scenarios

The NRC differentiates between two types of uncertainty, aleatory (variability) uncertainty and epistemic (state of knowledge) uncertainty. Epistemic uncertainties can be reduced by research (experimental or model development). Aleatory uncertainties cannot. The ultimate use of this study will be to assist in the prioritization of research activities. Thus, the focus is on epistemic uncertainties. Although there is variability (aleatory uncertainty) in design features among the different SFR designs under development, within the sensitivity study, the examination focused on only one specific plant design, as with the MST trial calculation described in Section 2. The belief is that there is sufficient similarity among industry designs that the issues and insights obtained would not substantially vary. Another potential source of variability is associated with different transient scenarios. For this reason, the same two transient scenarios chosen for the MST trial calculation were also utilized for the sensitivity calculation (although with slightly different characteristics):

- 1) **PLOF+**: It is assumed that over an extended period (*e.g.*, 2 days) the sodium pool heats up to 800°C. All the pins in the core are assumed to fail but there is no melting of fuel.
- 2) **UTOP+**: In this case, some melting of fuel occurs (1/3rd of core) but the primary sodium pool is at near-nominal temperatures.

Consideration must also be given to different modes of SFR operation, such as the burning of actinides extracted from LWR fuel or as a breeder reactor. The inventory of radionuclides in the fuel depends on the radiation history of the fuel. Typically, accident analyses are performed for the inventory at the end of an operating cycle, when the inventory is the largest. The inventory also depends on the mode of operation of the reactor. For this sensitivity study, two inventories were provided by Argonne analysts, one associated with an actinide burner mode of operation and the other for a breeder mode of operation.

3.1.2 Source Term Model

The model that was developed for this study should not be considered a MST analysis model. It does not perform a time-dependent analysis of accident phenomenology. Instead, it treats each of the stages of source term progression as consisting of independent first-order processes, in which removal rates by different processes, j , are represented by proportionality constants, λ_j . In common practice, the rate of leakage from a containment is treated in terms of fractional release rate per day, *e.g.* 0.1 volume percent per day. This is actually only true for conditions in which the containment pressure is sufficiently high such that the flow through the leak is choked and not a function of the pressure differential. At lower pressures, the leak rate is less than the “design” leak rate.

The model used in this study, which is described in Appendix B.1, uses design leak rates for the primary system leakage (except when primary system leakage is large) and for the containment leak rate. In a transient scenario, the containment pressure will be high for a limited period of time. For this study, it is assumed that the period of elevated pressure is 24 hours from the time at which fuel failure occurs. Material balance equations are developed for each stage of radionuclide transport, which are integrated over the 24-hour period. Radioactive decay is included in the base case analyses. Aerosol deposition is not considered within the cover gas region. Aerosol deposition is, however, included as a sensitivity study for the containment region for cases in which the primary system boundary is either not credited as a safety-grade boundary or for which primary system integrity is assumed to be lost as a consequence of the

accident conditions. In these cases, there could be substantial leakage of sodium to the containment atmosphere, sodium oxidation, aerosol production, aerosol agglomeration, and gravitational settling.

3.1.3 *Importance Measures*

Source terms are used in a variety of ways during the design process and in the licensing and regulatory oversight of nuclear power plants. Typically, TEDE is used as the human health response measure or is a significant contributor to the response measure for these applications. For example, as mentioned in Section 2.9.1, site dose calculations used to determine the exclusion area boundary and low population zone are based on a TEDE limit (25 rem over a specified time period). Comparisons with the NRC's Quantitative Safety Objectives are also based on TEDE for populations within zones in proximity of the plant [46]. For this reason, it is convenient for the purpose of the sensitivity study to develop a radionuclide importance measure that is proportional to TEDE, but does not require consideration of multiple meteorological scenarios.

A major insight obtained from the Fukushima accident is the relative importance of land contamination, relocation of members of the public, and decontamination costs following a radionuclide release. Although there are no direct U.S. regulations concerning land contamination following a radionuclide release, for the research prioritization conducted in Section 4, it is vital to ensure that radionuclides important to land contamination, but potentially of low importance to short-term dose, are not mistakenly excluded. Thus, for the purposes of this sensitivity study, it is also important to develop a measure that is directly associated with land contamination and relocation criteria.

It has been common practice in the development of source terms for licensing purposes or risk assessments to group different elements with common chemical behavior. However, the consequences of an environmental release depend on both the chemical properties and nuclear properties (half-life and mode of decay). For the sensitivity analysis, therefore, it is essential to examine the relative importance of the individual radionuclides rather than considering elemental groupings. In the actual applications of the MSTs, aggregation into groups with common elemental properties may be found to be of value.

Assessing the relative importance of a radionuclide begins with the inventory (curies). The inventory is then multiplied by a weighting factor to account for the relative health impact of exposure on a per curie basis. Four factors are then applied associated with the barriers to release: retention within fuel (complement of release fraction), retention within primary system comprised of retention within the sodium pool (taking into account capture within the pool and re-evolution of radionuclides to the cover gas region) as well as the potential to bypass the pool by transport in noble gas bubbles, retention within the cover gas region, and finally retention within the containment. To a large extent retention within the sodium pool and cover gas region of the primary system are coupled.

3.2 Source Term Decomposition

As discussed in the preceding section, in developing the NUREG-1465 alternative source term, it was found to be convenient to decompose the source term into constituent factors. This is also convenient for assessing the uncertainties associated with SFR source terms. There is a high level of defense-in-depth in an SFR associated with multiple barriers to the release of radioactive material to the environment. Although there are potential modes of release to the environment that involve other pathways for release of radioactive material to the environment, such as fuel handling accidents, failure of radioactive waste storage tanks, and containment bypass scenarios, that must be considered in a safety analysis report (SAR), the focus of this uncertainty and sensitivity analysis is accidents involving severe fuel damage including clad failure and the potential melting of fuel, release to the primary system sodium, release from the sodium pool to the cover gas region, release through the upper head of the primary vessel to a containment building and release from the containment building to the environment. It is convenient to decompose the release and transport analysis into four factors: release to sodium pool or bypass of the pool, release from sodium pool to cover gas region, release from cover gas region to containment and release from containment to the environment.

3.2.1 Radionuclide Weights

Historically, in major risk studies and in the development of alternative source terms, radionuclides have been aggregated into elemental groupings with common chemical characteristics, such as halides. For the purpose of this sensitivity study, the focus is on the behavior and importance of individual radioactive isotopes. Two weighting schemes have been examined. Analyses were performed using the NRC's RASCAL code, Version 4.3 [47]. In the first weighting scheme, 10^8 Ci of each radioisotope was released over a short time period and the dose was calculated at three miles with D stability meteorology and a wind speed of 5 meters per second. The calculation included inhalation dose from the passing cloud and 4 days of ground shine. This calculation was performed with ICRP26/30 dose conversion factors²⁶. Although meteorology and distance would have significant impact on absolute doses, the relative doses among different radionuclides are expected to be largely unaffected. The TEDE is the appropriate measure of exposure for site dose calculations, emergency response planning, and for evaluating conformance with probabilistic safety goals. For the noble gases, the external cloud shine controls the dose. For virtually all other radioisotopes, the inhalation dose is dominant.

Ingestion can be an important exposure pathway. In the Chernobyl accident, ingestion of iodine contaminated milk led to measurable increase in thyroid cancers among children in Ukraine and Byelorussia. However, the ingestion pathway is a controllable pathway, which for an open society concerned about the health of the public can be managed to assure minimal health impact. Historically, there has been high regulatory interest in radioactive iodine, in particular ^{131}I , because of the potentially high volatility of iodine in some fuel systems and the propensity for iodine to migrate to the thyroid, potentially leading to thyroid cancer. The TID-14844 source term is almost entirely focused on the release of radioactive iodine and noble gases, and limits the release of other elemental groups that would transport in the form of aerosols to one percent of the core inventory. As the following sensitivity studies show, radioactive iodine is less likely to be a dominant contributor to dose in SFR accidents. The other significant radiological impact of severe accidents is land contamination with the associated need for the relocation of people, loss of productivity, and expense of decontamination. Cesium isotopes, which are also major contributors to TEDE, are important contributors to the impact of land contamination because of their long half-lives and because they are gamma emitters.

²⁶ A comparison was made between ICRP26/30 and ICRP60 conversion coefficients. Although the weights are affected to some extent, they would have no impact on the insights gained from this study.

3.2.2 Release from Fuel

The principal references for assessing the mechanistic release and transport processes in this study of source term sensitivities are two Argonne reports: ANL-ART-3 [5] and ANL-ART-38 [6]. The release of radionuclides from the fuel matrix during normal operation, relocation within the fuel pin, and subsequent release are difficult to address on a first principles basis. There are significant uncertainties associated with chemical reactions among the radionuclides and the fuel matrix. There are, however, a number of experiments that have provided input to assessing the magnitude of release of the key radionuclides. Of particular importance is the change in morphology of the fuel associated with burnup. As described in Section 2.3.1, at moderate to high burnup levels, a network of interconnected porosity develops that results in substantial transport (up to 80 % of the noble gases to the upper and lower plena of the pins). A significant fraction of the cesium isotopes also escapes from the fuel matrix, and dissolves in the sodium bond, and migrate to the upper and lower plena. In contrast, the iodine radionuclides appear to largely remain within the fuel matrix during normal operation. Table 3-1 identifies the principal radionuclides, their inventory, the dose weighting factor, and the weighted dose for each isotope.

Table 3-1: Key Radionuclides - Example Burner Inventory and Radiological Weights²⁷

Isotope	Inventory	Weight	Weighted Inventory	Isotope	Inventory	Weight	Weighted Inventory
Am-241	2.92E+05	3.80E+06	1.11E+12	Pu-241	1.30E+07	7.10E+04	9.25E+11
Am-242	2.25E+07	5.00E+02	1.13E+10	Rb-86	1.22E+05	8.60E+01	1.05E+07
Ba-139	4.57E+07	2.00E+00	9.14E+07	Rh-105	4.42E+07	1.50E-01	6.62E+06
Ba-140	4.34E+07	2.50E+02	1.09E+10	Ru-103	5.44E+07	1.60E+02	8.71E+09
Ce-141	4.11E+07	9.00E+01	3.70E+09	Ru-105	4.42E+07	1.60E+01	7.08E+08
Ce-143	3.55E+07	5.40E+01	1.92E+09	Ru-106*	2.39E+07	4.20E+03	1.01E+11
Ce-144*	2.44E+07	3.20E+03	7.82E+10	Sb-127	3.41E+06	1.40E+02	4.78E+08
Cm-242	1.69E+07	1.50E+05	2.54E+12	Sb-129	1.02E+07	2.70E+01	2.76E+08
Cs-134	1.38E+06	6.80E+02	9.38E+08	Sr-89	1.41E+07	3.70E+02	5.22E+09
Cs-136	2.47E+06	4.00E+02	9.90E+08	Sr-90	8.90E+05	1.10E+04	9.79E+09
Cs-137*	2.60E+06	3.80E+02	9.87E+08	Sr-91	2.08E+07	4.40E+01	9.15E+08
I-131	1.07E+05	2.70E+03	2.89E+08	Sr-92	2.42E+07	2.30E+01	5.57E+08
I-132	4.25E+05	3.70E+02	1.57E+08	Tc-99m	4.30E+07	9.25E+00	3.97E+08
I-133	1.33E+06	3.20E+02	4.25E+08	Te-129	1.19E+06	1.20E+00	1.43E+06
I-134	7.12E+05	2.30E+01	1.64E+07	Te-129m	5.03E+05	2.30E+02	1.16E+08
I-135	1.22E+06	6.60E+00	8.03E+06	Te-131m	1.82E+08	1.70E+02	3.09E+10
Kr-83m	2.88E+07	3.40E+02	9.80E+09	Te-132	3.80E+06	3.70E+02	1.41E+09
Kr-85	4.11E+07	2.40E+01	9.87E+08	Xe-131m	3.00E+06	2.40E-02	7.21E+04
Kr-85m	5.42E+07	8.90E+01	4.82E+09	Xe-133	8.51E+07	1.00E-01	8.51E+06
Kr-87	5.82E+07	1.40E+01	8.15E+08	Xe-133m	3.33E+05	9.60E-02	3.19E+04
Kr-88	5.13E+07	4.60E+01	2.36E+09	Xe-135	4.28E+06	8.40E-01	3.60E+06
La-140	2.39E+06	1.60E+02	3.82E+08	Xe-135m	6.43E+04	7.90E-01	5.08E+04
La-141	1.37E+05	1.70E-02	2.34E+03	Xe-138	1.08E+06	4.30E+00	4.64E+06
La-142	4.50E+06	5.10E-01	2.29E+06	Y-90	9.44E+05	8.50E+01	8.02E+07
Mo-99	8.29E+06	2.70E+00	2.24E+07	Y-91	2.03E+07	4.30E+02	8.75E+09
Nb-95	1.05E+07	8.70E+00	9.10E+07	Y-92	2.45E+07	1.10E+01	2.69E+08
Nd-147	4.46E+07	2.40E+02	1.07E+10	Y-93	3.05E+07	2.50E+01	7.61E+08
Np-239	4.11E+07	6.50E+00	2.67E+08	Zr-95	3.69E+07	3.40E+02	1.26E+10
Pr-143	3.79E+07	1.90E+01	7.19E+08	Zr-97*	4.15E+07	8.30E+01	3.44E+09
Pu-238	4.90E+07	6.60E+01	3.23E+09				

The striking feature of the weighted inventories is how very large the weighted inventories are of the plutonium, americium, and curium isotopes in comparison with weighted inventories of other radionuclides. This is because of the very large inhalation dose associated with these alpha emitting radionuclides per curie inhaled. As will be shown later in this section, the overall importance of these radionuclides can be substantially reduced by factors associated with their transport and release to the environment.

²⁷Dose in rem at three miles per 10⁸ Ci.

In ANL-ART-38, bounding values for fuel release fractions are assessed for different elements based on a review of the existing database. The maximum expected fuel release fractions were assessed for four conditions: normal operation (500°C), eutectic formation (700°C), fuel melting (1100°C) and high temperatures (1300°C). Table 3-3 shows the assessed release fractions for the fuel melting condition and clad eutectic failure, which are representative of the two accident scenarios analyzed in this study.

Table 3-2: Upper Bound Radionuclide Release Fractions from Fuel

Fuel Conditions (Transient)	Xe/Kr	I	Cs	Eu	Te	Ba/Sr	Ru	La	Ce	Pu
<i>Eutectic Pin Failure (PLOF+)</i>	1.0	0.2	0.6	0.6	0.01	0.50	0.01	0.01	0.05	0.001
<i>Fuel Melting (UTOP+)</i>	1.0	0.3	1.0	1.0	0.05	0.65	0.05	0.3	0.1	0.001

3.2.3 Release from Sodium Pool

During normal operation, radionuclides released from the fuel matrix may transport through interconnected porosity to the gap region and to the upper and lower plena of the fuel pin where they may be dissolved in the sodium bond or react with the sodium bond. This is particularly true of cesium and europium. Following pin failure, the bubble of fission gases and any inert gas pre-pressurizing the pin will be rapidly released to the fuel channel. As will be discussed in Section 3.2.4, regarding bypass of the sodium pool, the effect of discharge of gas from the plena of fuel pins on flow in the channel, voiding of the channel, and the disruption of the column of liquid above a fuel channel are highly uncertain. However, the potential exists for some fraction of the radionuclides released from the fuel to be transported to the cover gas region without being captured in the pool.

Any radionuclides dissolved in the sodium bond material at the time of pin failure are likely to be carried with the sodium bond material and may be deposited in the sodium pool. If some fragmentation of the bond sodium occurs at the time of pin depressurization, the associated aerosols would be large and would be expected to be transported to the surface of gas bubbles and trapped in the pool by inertial forces. Depending on the chemistry of the radioisotopes released, they may dissolve in the sodium, react with the sodium or potentially be present in the form of small suspended particles, or they may react chemically with structures. At the upper surface of the pool there is a continual flux of sodium evaporating from the pool into the cover gas region and a continual flux of sodium vapor returning to the pool. If the cover gas region remains intact, an equilibrium is established. If there is a significant pathway for release through the head region, sodium vapor and gases in the cover gas region can escape to the containment region, carrying radioactive material with it. If the leakage path to the containment is small, the offsite consequences of the accident will be minor. The larger the leak path, the greater the net vaporization of sodium from the pool and the greater the net vaporization of dissolved radionuclides from the pool. In the report ANL-ART-3, relative fractional releases of key elements are compared with the fractional release of sodium. By examining these data at low fractional sodium release levels, coefficients were developed for the fractional release of each elemental group for a given fractional loss of sodium from the pool, as presented in Table 3-3.

Table 3-3: Fractional Release Relative to Fractional Release of Sodium

Pool Temperature	Cs	I	Rb	Te	Sr	Ba	Eu¹
1100 K	34	0.2	19	0.065	0.013	0.003	2.4E-3
800 K	120	0.13	50	0.025	0.028	-	3E-5

¹Based on Raoult's Law

Raoult's law (Eq. 1) relating the relative releases of solute materials to the relative vapor pressures of pure substances can be used to bound the release of the solute material. This approach was used to extend Table 3-3 to other elemental groups as designated in the table.

$$p_{ig} = \hat{p}_{lg} X_{i,cond} \quad \text{Eq. 1}$$

where,

p_{ig} = vapor pressure of component i in cover gas region

$\hat{p}_{lg}$ = saturated vapor pressure of component i

$X_{i,cond}$ = mole fraction of component i in condensed phase

Based on Raoult's Law there would be effectively no release of either the americium group or plutonium group of radionuclides by evaporation from the sodium pool. In performing the sensitivity study, it must be recognized that there are other potential mechanisms for the release of radioactive material from the pool beyond evaporation, as described in Section 2.6.1. Since the purpose of this sensitivity study is to identify those radionuclides and mechanisms that have the greatest impact on offsite dose, it is possible to use a bounding value for those unanalyzed mechanisms.

In the sensitivity study, two principal parameters are examined: fraction of failed fuel and percent sodium released to the containment. Two radioactive isotopes of sodium, ^{22}Na and ^{24}Na , are created during normal operation as the sodium is irradiated by neutrons as it flows through the core. Based on design values for past Argonne SFR designs [48], importance of the release of these radionuclides in assessing the relative importance of radionuclides in the sensitivity study has been examined. The expected operational activity level of ^{24}Na is 11.2 Ci/kg and of ^{22}Na is 1.1E-3 Ci/kg. Knowing the mass of sodium in the primary system, it is possible to calculate the total radioactive sodium inventory. However, in the analysis of sodium retention and evaporation conducted here, it assumed that only half of the liquid sodium in the pool is associated with the release to the cover gas region. If there is substantial fuel damage and release of cesium isotopes to the pool, the contribution of the sodium isotopes to the release to containment will be negligible relative to the release of cesium isotopes, in part because of the higher fractional release of cesium per percent sodium release and the higher dose weighting factors for the cesium isotopes relative to the weighting factors for the sodium isotopes.

3.2.4 Bypass of Sodium Pool

During normal operation, the release of noble gas fission products to the plenum region of the fuel pin leads to a substantial increase in the internal pressure of the pin. If fuel pins fail during a transient, which is likely to occur near the top of the fuel column, the gases in the fuel pin will expand and expel the bond sodium above the fuel column (which can contain radionuclides released from the fuel during operation). The released gases, which contain radionuclide vapors and aerosols, can expand across multiple pins within an assembly. If expanded to atmospheric pressure, the volume of gases released from an assembly would be greater than the volume of sodium in the 10 meter-high column directly above the fuel assembly. Thus, it appears likely that failure of fuel pins will lead to extreme turbulence and mixing of the pool, as well as pressurization of the cover gas region. It is difficult to model the capture of aerosols and radionuclide vapors that would occur in this phase of the accident.

Argonne staff have developed a bubble transport model to assess the fraction of aerosols captured in the pool. The equations for diffusion, inertial deposition, diffusiophoresis, thermophoresis and gravitational settling within a bubble are well known mechanisms [20]. The size of the bubble can be assessed from stability considerations and the rise velocity of the bubble related to its size. However, when taking into account non-spherical bubble geometry, induced flow patterns within the bubble, and mechanisms affecting bubble formation and breakup there is significant uncertainty associated with the assessment of decontamination factors. Furthermore, it is not clear how applicable an isolated bubble model is to the time period immediately following pin failure or during later stages of an accident in which radionuclides continue to be evolved. At the time of pin failure, the released gases may appear more like a jet than a

bubble depending on the characteristics of pin failure. The volume of released gases may rapidly break into a swarm of smaller bubbles in the open sodium pool region above the core. There is inadequate modeling and validation of the conditions associated with this phase of an accident to accurately assess the associated decontamination factors. It is clear, however, that pool temperature relative to the initial conditions in the bubble has a major impact on the magnitude of decontamination factors, associated with diffusiophoretic and thermophoretic effects. For the purposes of this study, bypass of the pool is treated parametrically using results of Argonne bubble transport analyses to represent the lower end of bypass fraction.

When the bubble breaks the surface of the sodium pool, some of the liquid sodium at the surface of the bubble can be aerosolized as a splash which can carry radioactive material into the cover gas region in the released droplets. The sensitivity model does not explicitly include this contribution to bypass.

Many radionuclides are released as vapors from over-heated fuel. Whether they are in an elemental form or have reacted with other chemicals to form compounds depends on chemical kinetics and timing. Best estimates of the chemistry of the released vapors can be made using chemical thermodynamic equilibrium codes. The results of these analyses can provide insights but are not definitive. As the released vapors move toward colder regions within a fuel pin, the vapors will condense to form aerosols depending on their vapor pressure relative to the saturation pressure at that temperature. Released radionuclides may condense homogeneously within the vapor space of the fuel pin or heterogeneously onto other aerosols or surfaces. Condensed aerosols are typically very small, *e.g.* on the order of 0.1 micron. This happens to be near the minimum of the curve of decontamination factor (DF) as a function of aerosol size that is most likely to transport to the surface of the sodium pool in bubbles without being captured in the pool [49].

3.2.5 Release from Cover Gas Region

Radionuclides reach the cover gas region either by evolving from the pool, which is treated in the sensitivity model as occurring in proportion to sodium evolution, or by bypassing the sodium pool. It is assumed that the system is designed with primary system boundary as a safety grade system with a design release rate of 0.1 v/o per day at a specified pressure. In the analysis model, no credit is given for retention of aerosols or vapors on structures within the cover gas region. For the case studies discussed in Section 3.4, consideration is given to two cover gas region leakage conditions. In one set of base cases, the cover gas region leaks into the containment region at the specified leak rate for the duration of the event. The partial pressure of sodium vapor is maintained at the saturation pressure (at the pool temperature) by net evaporation. The amount of radionuclide release of species that volatilize from the pool is proportional to the leakage of sodium.

In another set of base cases, it is assumed that the integrity of the cover gas region is compromised, such that a substantially larger leakage of sodium occurs to the containment. This can also be considered a design variation in which the primary system is not credited as a low leakage barrier. Again, the leakage to containment of other radionuclides is proportional to the sodium loss from the pool. For the PLOF+ scenario with a high pool temperature (830°C) a total leakage of 1% of the upper pool sodium is assumed. At 830°C, the evaporation rate of sodium into an open containment is approximately 30 kg/m²-hr [50], which could easily result in a release of 1% over a 24 hour period. At 530°C, the release rate into an open containment is only approximately 0.8 kg/m²-hr, which corresponds to slightly less than 0.5% over a 24-hour period. For this reason, in the UTOP+ scenario with a failed primary system the total leakage of sodium is limited to 0.5%.

3.2.6 Release from Containment

The final barrier for release of radionuclides to the environment is the reactor containment. It is expected that the SFR designs will use traditional, essentially leak tight containments, even though the expected

consequences without containment might satisfy regulatory criteria for offsite doses. For the current study, a comparatively high design leak rate of one volume percent release per day is assumed. Assessing the sensitivity to containment leak rate can be determined using a multiplicative factor proportional to the leak rate. By delaying release to the environment, the containment allows time for radioactive decay and for deposition mechanisms, such as gravitational settling, inertial deposition, and thermophoresis to capture aerosols and prevent their release to the environment. The analysis of containment transport and deposition of aerosols is comparatively well-developed. Considerable research effort was dedicated to this area early in the fast reactor development program, including methods development and validation for the treatment of multi-aerosol sources [51]. Some expertise and judgment is required in exercising these models, such as in the identification of shape factors. There are also some residual areas of remaining uncertainty, such as charge effects arising from radioactive decay of aerosol constituents.

3.2.7 *Consequence Metrics*

The dose weighted consequences obtained with the analysis model are intended to illustrate the relative contribution of different radionuclides to the dose (TEDE) to which a member of the public would be exposed, regardless of distance from the plant or meteorology. The model specifically calculates the inhalation dose, cloudshine, and 4-day groundshine to which an individual would be exposed at 3 miles from the plant for D meteorology and a 5 mph wind speed times a normalizing factor of 1×10^8 .²⁸ Using dose conversion factors obtained from RASCAL analyses associated with one year of groundshine, the sensitivity model also calculates the one-year groundshine dose, again multiplied by a normalizing factor of 1×10^8 . To provide some perspective on whether the total doses are large or small relative to regulatory criteria, approximate conversion factors are used to translate the results of the case studies to regulatory applications, specifically those addressing site dose criteria and emergency planning criteria.

The site dose criteria, described in Section 3.1.3, limit the dose at the boundary of the exclusion area to 25 rem for the worst two hours of the event and at the boundary of the low population zone to 25 rem over the duration of the event. These calculations are performed for site specific conservative meteorology (95th percentile). From the Gaussian dispersion equation for the transport of radionuclides, the term χ/q (airborne concentration of a radionuclide per unit source at the location of interest) is used to characterize a site based on local meteorology. It is an objective of advanced reactors to substantially reduce the size of the site boundary and emergency planning zone. To provide some perspective on the severity of releases, the dose at 200 meters from the release point is provided by adjusting the 3-mile dose value by the associated χ/q value. The reader should recognize that a detailed analysis for a specific site would be required to obtain an accurate site dose value. This value represents a low population zone dose at this distance. With the simplified model used in this study, doses during the first two hours tend to be small because of the time required for radionuclide concentration to build up in the containment. Similarly, a total one-year groundshine dose is calculated at the 3-mile location. The results of this analysis can be compared to the 2 rem limit in the first year of exposure used to determine whether people would be required to relocate, as part of the U.S. Environmental Protection Agency's Protective Action Guides [52]. Again, these benchmarks are only provided for perspective.

²⁸ The output of RASCAL does not use scientific notation. To obtain conversion coefficients to be used as weighting factors, 1×10^8 curies of each radionuclide was released to yield measurable doses in the RASCAL output. Thus, the weighting factors are based on a calculated dose per 10^8 curies of isotope released.

3.3 Case Studies

The base cases address aleatory variability associated with some design considerations, two characteristic scenarios, and two operational modes. The base cases are performed with assumptions associated with the conservative end of the range of epistemic uncertainty. Sensitivity studies, described in Section 3.4, are subsequently performed to determine the potential reduction in source terms associated with improved modeling and model validation. The base case studies are identified in Table 3-4. Table 3-5 provides approximate measures of regulatory significance for each of the base cases. The following subsections will describe each base case in further detail.

Table 3-4: Sensitivity Calculation – Case Studies

Case Study	Operating Mode	Transient	Fuel Failure (% of total core)	Pool Temp. (°C)	Primary Leakage	Pool DF
1	Burner	PLOF+	100%	830	0.1 v/o	3
2	Burner	PLOF+	100%	830	1% Sodium	3
3	Burner	UTOP+	33%	530	0.1 v/o	10
4	Burner	UTOP+	33%	530	0.5% Sodium	10
5	Breeder	PLOF+	100%	830	0.1 v/o	3
6	Breeder	PLOF+	100%	830	1% Sodium	3
7	Breeder	UTOP+	33%	530	0.1 v/o	10
8	Breeder	UTOP+	33%	530	0.5% Sodium	10

Table 3-5: Case Study Overview – Regulatory Dose Perspective

Case Number	Scenario Description			Offsite Consequence (rem)		
	Transient	Type	Primary System Boundary	Total Dose ¹ (3 Miles)	Total Siting Dose ¹ (200m)	Total 1 Yr Groundshine Dose ² (3 Miles)
1	PLOF+	Burner	Intact	8.7E-4	0.29	1.1E-3
2	PLOF+	Burner	Degraded	1.8	490	2.0
3	UTOP+	Burner	Intact	2.9E-3	0.71	4.3E-4
4	UTOP+	Burner	Degraded	5.8	1500	1.6
5	PLOF+	Breeder	Intact	8.0E-4	0.21	1.2E-3
6	PLOF+	Breeder	Degraded	1.3	340	2.0
7	UTOP+	Breeder	Intact	1.8E-3	0.47	3.9E-4
8	UTOP+	Breeder	Degraded	3.5	940	1.6

¹ Compared to 25 rem

² Compared to 2 rem

3.3.1 Case Study 1: PLOF+ - Burner Reactor

Figure 3-1 shows the Case 1 dose-weighted results for the top 21 isotopes²⁹. On a logarithmic scale, the product of factors appears as additive terms. Thus, it is easy to deduce visually what factors are most important. The use of dose-weighted source terms is intended to provide a relative mechanism for comparing source terms on a common basis with regard to their potential dose impact. Some insights obtained from this case are:

- 1) The alpha emitters, ²⁴²Cm, ²⁴¹Am, and ²³⁸Pu, dominate the dose because of their high weighting factors, despite their relatively low release fractions from the fuel. ¹⁴⁴Ce is also a significant contributor. The pool has very little effect on these radionuclides for this case study because of the high degree of pool bypass assumed.

²⁹ Complete results presented in Appendix B.2.

- 2) The length of the bar from the yellow circle to the bright orange circle indicates the importance of primary system retention, which as expected for a 24-hour accident and a release rate of 0.1 v/o per day is a factor of 1000. The containment retention factor (length of the bar from the red circle to the red diamond) is typically on the order of 500 or greater. This is in part because of the release rate from containment of 1 v/o per day but also because of the delay imposed by the primary system for radionuclides entering the containment and the added time for radioactive decay.
- 3) Most of the noble gases have short half-lives. As a result, only ^{83m}Kr (37^{th} on the list) remains a significant contributor to offsite dose. The weighted inventory and release to the cover gas region are essentially identical because the release from the fuel is effectively 100 percent.
- 4) The ^{131}I release has higher contribution to the dose than the cesium isotopes because of the higher inventory and because of the high bypass fraction. The cesium isotopes are primarily captured in the sodium pool and because there is little leakage of sodium vapor to the containment, the cesium largely remains in the pool.
- 5) ^{140}Ba and ^{90}Sr rank surprisingly high. Whether a fifty percent release fraction from the fuel is appropriate for a low temperature (eutectic failure) release likely requires further investigation.

Figure 3-1: Case Study 1 – Principal Dose Contributors

Figure 3-2 illustrates the contribution of the key radioisotopes to the 1-year groundshine dose. The high importance of the cesium isotopes is no surprise. The large impact of ^{140}Ba is surprising but could reflect an overestimation of the fuel release fraction.

Figure 3-2: Case Study 1 – Land Contamination

3.3.2 Case Study 2: PLOF+, Degraded Primary System - Burner Reactor

This case study can either be considered a variation in plant design in which the primary system boundary does not have a controlled leak rate, or a variation in scenario in which the primary system boundary fails during the transient. In this scenario, there is substantial leakage of sodium (1% of the upper pool mass), which leaks into the containment. Because the pool is at high temperature, sodium evaporates rapidly from the pool. Radionuclides captured in the pool evaporate in proportion to the fractional release of sodium. In these scenarios, sodium entering the containment would react with the oxygen and moisture content of the containment atmosphere. No credit is given to aerosol deposition in the containment in this case study. Figure 3-3 shows the ranking of key radionuclides for this case (complete results in Appendix B.2).

Figure 3-3: Case Study 2 – Principal Dose Contributors

The absolute values of the doses are substantially higher for this case relative to the case in which the primary system is intact. However, there are only minor differences in the ranking of the isotopes. Some europium isotopes have increased significance for this case. Although there is more contribution to the containment source term from radionuclides evolved from the sodium pool because of the large bypass fraction, evolution from the pool does not have a major impact on the consequences. Figure 3-4 provides the results for 1 year of groundshine. In this case, the evolution of sodium from the pool results in a clear dominance of the groundshine dose by cesium isotopes.

Figure 3-4: Case Study 2 – Land Contamination

Table 3-5, at the beginning of this section, indicates the importance of primary system integrity as it affects the severity of the environmental release. The 1 year groundshine dose of 2 rem for this case indicates the likelihood that in this type of scenario, some relocation of members of the public could be required. The 200 meter dose is substantially higher than what would be acceptable for the low population zone.

3.3.3 Case Study 3: UTOP+ - Burner Reactor

For the UTOP+ scenario, although 1/3 of the fuel is damaged, it is assumed that these assemblies contain ½ the inventory of the core, due to higher burnup levels. Because of the higher fuel temperatures, the release fractions from the fuel are higher than for the PLOF+ accident. However, the pool is cooler, reducing releases to the cover gas. Figure 3-5 illustrates the relative importance of the different radionuclides to offsite dose. In comparison with Figure 3-1, which relates to the PLOF+ accident, the relative importance of the principal radionuclides are not substantially different. The alpha emitters with high inhalation doses dominate the consequences. Figure 3-6 illustrates the relative contributions for land contamination. In comparison with Case Study 1, there are only minor differences in the rankings of radionuclides relative to their contribution to the 1 year dose.

The UTOP+ accident is expected to be a more severe accident than the PLOF+ accident because the temperatures reached by the fuel are higher. From Table 3-5, the offsite dose is approximately a factor of three higher, but still without substantial offsite consequences. Perhaps surprisingly, the extent of land contamination is actually smaller than for the PLOF+ accident. This is because the partial pressure of sodium in the cover gas region is substantially higher in the PLOF+ accident, leading to a greater release of cesium and barium isotopes to the containment and to the environment. In addition, only 50% of the core inventory is associated with failed fuel.

³⁰ For the isotopes of cesium, 100% of the fuel inventory is released (resulting in overlapping points on the plot).

3.3.4 Case Study 4: UTOP+, Degraded Primary System - Burner Reactor

This scenario is expected to have the most severe consequences of the four studied, due to the larger release fractions from the damaged fuel and the degraded primary boundary. Figure 3-7 illustrates the relative importance of the principal radionuclides to offsite dose and Figure 3-8 illustrates the importance to land contamination and the potential need for relocation of members of the public. As Table 3-5 indicated, in comparison with Case Study 2, the offsite doses are approximately a factor of three higher (the same ratio is true for case studies 1 and 3). This scenario would clearly not satisfy the low population zone criterion at 200 meters. The 1 year dose from groundshine at three miles is slightly less than the EPA protective action requirement for relocation.

Figure 3-7: Case Study 4 – Principal Dose Contributors

Figure 3-8: Case Study 4 – Land Contamination

3.3.5 Breeder Reactor Inventory Case Studies

Cases 1 through 4 were repeated utilizing a breeder core inventory, rather than an actinide burner. Table 3-6 shows the difference between the burner and breeder inventories for the principal radionuclides. The differences are small, generally on the order of 20% with a maximum difference of a factor of two for ²⁴²Am. Because the inventories are so similar, the insights obtained for these case studies are essentially the same as for the burner fuel case studies, and a detailed description of each breeder case study is not provided here (complete results can be found in Appendix B.2). As indicated in Table 3-5, the assessed consequences of scenarios with the burner fuel are slightly higher than those of the breeder core consistent with the somewhat higher inventories, particularly of the actinide isotopes.

Table 3-6: Comparison of Breeder and Burner Core Inventories

<i>Isotope</i>	<i>Burner/Breeder Ratio</i>	<i>Isotope</i>	<i>Burner/Breeder Ratio</i>	<i>Isotope</i>	<i>Burner/Breeder Ratio</i>
<i>Am-241</i>	<i>1.37</i>	<i>Kr-88</i>	<i>1.21</i>	<i>Sr-91</i>	<i>1.17</i>
<i>Am-242</i>	<i>2.02</i>	<i>La-140</i>	<i>1.17</i>	<i>Sr-92</i>	<i>1.18</i>
<i>Ba-139</i>	<i>1.22</i>	<i>La-141</i>	<i>0.85</i>	<i>Tc-99m</i>	<i>1.20</i>
<i>Ba-140</i>	<i>1.21</i>	<i>La-142</i>	<i>1.17</i>	<i>Te-129</i>	<i>1.19</i>
<i>Ce-141</i>	<i>1.21</i>	<i>Mo-99</i>	<i>1.17</i>	<i>Te-129m</i>	<i>1.19</i>
<i>Ce-143</i>	<i>1.21</i>	<i>Nb-95</i>	<i>1.17</i>	<i>Te-131m</i>	<i>1.17</i>
<i>Ce-144*</i>	<i>1.07</i>	<i>Nd-147</i>	<i>1.24</i>	<i>Te-132</i>	<i>1.20</i>
<i>Cm-242</i>	<i>1.87</i>	<i>Np-239</i>	<i>1.21</i>	<i>Xe-131m</i>	<i>1.20</i>
<i>Cs-134</i>	<i>1.02</i>	<i>Pr-143</i>	<i>1.21</i>	<i>Xe-133</i>	<i>1.16</i>
<i>Cs-136</i>	<i>1.25</i>	<i>Pu-238</i>	<i>1.20</i>	<i>Xe-133m</i>	<i>1.19</i>
<i>Cs-137*</i>	<i>0.86</i>	<i>Pu-241</i>	<i>1.63</i>	<i>Xe-135</i>	<i>1.21</i>
<i>I-131</i>	<i>0.98</i>	<i>Rb-86</i>	<i>1.19</i>	<i>Xe-135m</i>	<i>1.20</i>
<i>I-132</i>	<i>0.97</i>	<i>Rh-105</i>	<i>1.23</i>	<i>Xe-138</i>	<i>1.22</i>
<i>I-133</i>	<i>1.32</i>	<i>Ru-103</i>	<i>1.21</i>	<i>Y-90</i>	<i>0.84</i>
<i>I-134</i>	<i>1.33</i>	<i>Ru-105</i>	<i>1.23</i>	<i>Y-91</i>	<i>1.16</i>
<i>I-135</i>	<i>1.37</i>	<i>Ru-106*</i>	<i>1.08</i>	<i>Y-92</i>	<i>1.18</i>
<i>Kr-83m</i>	<i>1.19</i>	<i>Sb-127</i>	<i>1.18</i>	<i>Y-93</i>	<i>1.18</i>
<i>Kr-85</i>	<i>1.20</i>	<i>Sb-129</i>	<i>1.19</i>	<i>Zr-95</i>	<i>1.18</i>
<i>Kr-85m</i>	<i>1.20</i>	<i>Sr-89</i>	<i>1.16</i>	<i>Zr-97*</i>	<i>1.20</i>
<i>Kr-87</i>	<i>1.21</i>	<i>Sr-90</i>	<i>0.83</i>		

3.4 Sensitivity Studies

The eight base case studies described in Section 3.3 are intended to represent major sources of variability (aleatory uncertainty) associated with plant design features, modes of plant operation, and characteristic accident scenarios. However, the analysis of epistemic uncertainty more directly addresses the question of what additional research is required and those aspects of the analysis for which research can be most effective. A number of sensitivity studies have been undertaken relative to the base cases associated with the range of the principal elements of epistemic uncertainty as identified in Table 3-7, with regulatory dose perspective summarized in Table 3-8. Other sensitivity studies can be performed by simply perturbing the results of the base cases, as will be described in subsequent subsections.

Table 3-7: Sensitivity Study Case Matrix

Case	Scenario Description					
	Type	Transient	Ac/La Fuel Release	Aerosol Deposition	Primary Leakage	Pool DF
1.1	Burner	PLOF+	Nom – 0.1%	Nom - No	Nom - 0.1 v/o	30
2.1	Burner	PLOF+	Nom – 0.1%	Nom - No	0.5% Sodium	30
3.1	Burner	UTOP+	Nom – 0.1%	Nom - No	Nom - 0.1 v/o	1000
4.1	Burner	UTOP+	Nom – 0.1%	Nom - No	1% Sodium	1000
2.2	Burner	PLOF+	Nom – 0.1%	Yes ($\lambda = 3E-5$)	0.5% Sodium	Nom - 3
4.2	Burner	UTOP+	Nom – 0.1%	Yes ($\lambda = 3E-5$)	1% Sodium	Nom - 10
2.3	Burner	PLOF+	0.0001%	Nom - No	1% Sodium	Nom - 3
4.3	Burner	UTOP+	0.001%	Nom - No	0.5% Sodium	Nom - 10

¹Ac/La – Actinide/Lanthanide

Table 3-8: Sensitivity Study – Regulatory Dose Perspective

Case	Offsite Consequence (rem)		
	Total Dose ¹ (3 Miles)	Total Siting Dose ¹ (200m)	Total 1 Yr Groundshine Dose ² (3 Miles)
1.1	1.1E-4	0.030	2.0E-4
2.1	0.21	56	0.72
3.1	2.9E-5	7.6E-3	4.9E-6
4.1	0.1	13	0.85
2.2	0.67	178	0.79
4.2	0.1	13	0.85
2.3	0.37	98	1.9
4.3	0.30	84	1.6

¹ Compared to 25 rem

² Compared to 2 rem

3.4.1 Sodium Pool Bypass

The first sensitivity study conducted examined the importance of the pool decontamination factor (bubble scrubbing). The decontamination factor (DF) was increased by a factor of 10 for the PLOF+ case (from 3 to 30), and by a factor of 100 for the UTOP+ case (from 10 to 1000). Complete results can be found in Appendix B.3. Based on the indicators of regulatory significance described in Table 3-9, importance measures can be developed in terms of ratio of the initial value of the dose over the perturbed value of the dose associated with the potential benefit of research. Because the pool is cold relative to the gases released from the fuel, the importance of pool decontamination is greater for the UTOP+ transient than for the PLOF+ scenario. The reason that the dose reduction factor for the UTOP+ with the failed primary system is comparatively small is that the land contamination dose is dominated by cesium isotopes in the base case and the release of cesium isotopes is controlled by evolution from the pool rather than bypass fraction.

Table 3-9: Hot Pool Bypass Sensitivity Results

Case	Transient	Dose Reduction Factor	
		Site Dose	Land Contamination
1.1	PLOF+	7.7	5.5
2.1	PLOF+, Degraded Primary	8.6	2.8
3.1	UTOP+	100	88
4.1	UTOP+, Degraded Primary	58	2

3.4.2 Containment Aerosol Deposition

For those scenarios in which the primary system remains intact, aerosol concentrations and vapor forms of radionuclides (to the extent they exist) would be small. Although these concentrations would be reduced by natural deposition mechanisms, it is unlikely there would be orders of magnitude reductions. Radioactive decay and loss of a driving force for release reduce the long term release of radioactive material to the environment. For this reason, the two cases examined in the containment deposition sensitivity study involve failure of the primary system and a large release of sodium vapor to the containment where it will react with moisture and oxygen to produce aerosols. Radionuclides released to the containment will produce aerosols that co-agglomerate with the sodium oxide aerosols and are effectively removed from the containment atmosphere primarily by gravitational settling. Table 3-10 contains the importance results. The aerosol removal rate was based on fitting the results of experiments performed by HEDL under conditions quite similar to the aerosol loadings for these cases [51].

Table 3-10: Containment Aerosol Sensitivity Results

Case	Transient	Dose Reduction Factor	
		Site Dose	Land Contamination
2.2	PLOF+, Degraded Primary	2.7	2.6
4.2	UTOP+, Degraded Primary	2.8	2.3

3.4.3 Actinide/Lanthanide Fuel Release Fractions

The upper bound fuel release fractions provided in ANL-ART-38 for some of the low volatility elements in the lanthanide and actinide regions of the periodic table are sufficiently large that these elements have a significant impact on consequences. Without a complete understanding of the chemical compounds formed among the low volatility fission products, it is difficult to dismiss them as insignificant contributors to offsite dose merely on the basis of the equation of state of the elemental form. Nevertheless, it is quite possible that the best estimate release fractions based on additional experimental information could be reduced substantially relative to these bounding values. In this sensitivity study, the fuel release fractions for the lanthanide and actinide groups are set as 1E-4 for the eutectic failure release level (800 °C) and to 1E-3 for the fuel melting release level (1100 °C). In reality, realistic fuel release fractions could be lower than these sensitivity study values, but it is very difficult to demonstrate very small release fractions experimentally. The complete results, found in Appendix B.3, show that the reduction of the fuel release fractions directly impacts the dose measures and significantly affects the ranking of radionuclides. Table 3-11 identifies the dose reduction importance measures associated with the fuel release fraction sensitivity study. The potential impact on site dose assessment is quite large. There is virtually no impact on land contamination, because actinides and lanthanides have no impact on the groundshine dose received in the first year (although they can affect a long term inhalation dose associated with their resuspension).

Table 3-11: Actinide/Lanthanide Fuel Release Sensitivity Results

Case	Transient	Dose Reduction Factor	
		Site Dose	Land Contamination
2.3	PLOF+, Degraded Primary	4.9	1.1
4.3	UTOP+, Degraded Primary	19	1

3.4.4 Distribution of Radionuclides within, and Evolution from, the Sodium Pool

The discussion of pool bypass is directly relevant to the uncertainties associated with the capture by the pool of radionuclides released from the fuel. Modeling the flow of sodium from the outlet of the core to the pool surface and recirculation back to the inlet the reactor would require computationally intensive computational fluid dynamic analysis. Tracking radionuclide concentrations throughout that flow regime is a daunting problem, particularly since it is not clear whether radionuclides are associated with captured aerosols, are in solution in their elemental form, or have reacted with sodium or with other fission products. Except for a few elements (and compounds) assessing the partitioning between radionuclides in solution with radionuclides in vapor form in the cover gas region is also uncertain. In this analysis, the concentration of radionuclides near the surface of the pool has effectively been increased by assuming that the radionuclides are dissolved in only $\frac{1}{2}$ of the mass of the sodium pool. The results of the sensitivity study performed indicated that the questions associated with the evolution of radionuclides from the pool only significantly affects cesium release. However, if additional research indicates that decontamination factors for the pool are significantly higher than currently believed, the substantial uncertainties associated with radionuclide distribution in the pool and evolution of radionuclides from the pool to the cover gas region will become more significant.

3.4.5 Containment Leak Rate

The sensitivity studies were performed for a design leak rate of 1 v/o per day, which is larger than typical for LWRs. However, the combination of a leak-tight primary system and a comparatively large containment design leakrate are effective in limiting the release of radionuclides to the environment. Nevertheless, the source term is approximately proportional to the containment leak rate. The releases to the environment in the cases examined would be a factor of ten smaller with a design leak rate of 0.1 v/o per day. In fact, typically plant operators select their design leak rate to satisfy the 25 rem site boundary dose limits (with some cushion to account for potential regulatory issues), because of the operating penalty associated with periodically demonstrating compliance with the plant's design leak rate. The more stringent the design leak rate, the more costly the effort to demonstrate compliance.

3.4.6 Noble Gas Decay Chains

Typically, source term analyses do not model the effects of radioactive decay chains when considering the transport of radionuclides from the fuel to the environment. In particular, some noble gases could potentially be released with high release fractions from the fuel, bubble through the sodium pool, and then decay into other elemental radionuclides with significantly higher radiological impact. To assess the potential contribution to the offsite dose, an analysis was made of the impact on Case Study 1, PLOF+ with high pool bypass. A comparison is made between the predicted amount of the daughter isotope transported to the cover gas region with the amount that would arise from the parent transporting to the cover gas region as a noble gas. Table 3-12 shows the fractional contribution associated with transport of the parent noble gas to the assessed value for the daughter isotope. A comparison is also made with the overall weighted source term to the cover gas region. In all cases, the contributions are small. For Case Study 1, the DF of the pool is small. For cases in which a higher DF can be justified, the potential contribution from noble gas parents could be greater. However, based on the results obtained, it appears unlikely that including radionuclide chains would be a necessary aspect of a mechanistic source term

methodology based only on the need to consider noble gas transport and subsequent decay into radionuclides with higher radiological significance.

Table 3-12: Contribution From Noble Gas Parent Assessment

<i>Parent</i>	<i>Daughter</i>	<i>Fractional Contribution to Daughter Source Term</i>	<i>Fractional Contribution to Overall Dose-Weighted Source Term</i>
⁹¹ Kr	⁹¹ Sr	2.3E-4	8.6E-6
⁹² Kr	⁹² Sr	2.5E-8	1.6E-10
⁹³ Kr	⁹³ Y	7.8E-4	8.5E-8
¹³⁷ Xe	¹³⁷ Cs	2.2E-5	1.9E-7
¹³⁹ Xe	¹³⁹ Ba	3.0E-2	2.0E-5
¹⁴⁰ Xe	¹⁴⁰ Ba	3.0E-5	2.4E-6

3.5 Findings

The sensitivity studies performed in Section 3.4 categorized the importance of several main modeling areas, shown in Table 3-13. This includes two major areas of uncertainty that could substantially influence source term analyses: sodium pool decontamination factors (bypass) and fuel release fractions for actinide and lanthanide radionuclides. The remainder of this section discusses these phenomena areas in further detail.

Table 3-13: Importance Assessment from Sensitivity Study

<i>Phenomena</i>	<i>Importance</i>
<i>Pool Bypass (Bubble Transport)</i>	<i>Very High</i>
<i>Fuel Release Fractions (Actinide/Lanthanide)</i>	<i>High</i>
<i>Aerosol Deposition/Removal</i>	<i>Medium</i>
<i>Reactor Head/Containment Leak Rate</i>	<i>Medium</i>
<i>Pool Vaporization</i>	<i>Low</i>
<i>Noble Gas Decay Chains</i>	<i>Low</i>

Pool Bypass (Bubble Transport)

The area that stands out as the highest priority in the sensitivity studies is the assessment of pool bypass. Although there is some ongoing work at Argonne related to bubble transport, with the current state of knowledge, it is unclear whether the transport of isolated bubbles provides a realistic characterization of bypass conditions. Of particular concern are the conditions associated with the failure of fuel pins, the discharge of gases, vapors, aerosols and bond sodium at high pressure into the fuel channel and the area of the pool above the fuel assembly. The high degree of turbulence induced in the pool could significantly impact the retention or transmission of radioactive material. To a significant extent, the study of these phenomena can be performed with simulants.

Fuel Release Fractions of Actinides and Lanthanides

Lacking further information, americium, curium, and plutonium isotopes appear to dominate SFR source terms. It is quite possible that the bounding fuel release fractions that lead to this conclusion are too conservative. The cost of the type of prototypic experiments required to improve estimates of release fractions is high. However, in the performance of those experiments it should also be possible to improve estimates of fuel release fractions for all of the other important radionuclides as well. In addition, there is a need for a mechanistic fuel source term model capable of modeling changes in fuel morphology with burnup, the relocation of radionuclides during power plant operation, and release rates of radionuclides as a function of time and temperature in an accident, including an assessment of radionuclide chemistry. Model development and experimental design, as a basis for model validation, should be tightly coordinated. Much of the technical basis for model development already exists.

Aerosol Deposition/Removal and Reactor Head/Containment Leak Rate

The inclusion of containment aerosol retention mechanisms is important, although considered of *medium* importance compared to the impact of the first two gap areas. However, this is an area in which there has already been considerable research and models do exist. Reactor head/containment leakage are also important, but their impact is of direct proportion to leakage rate. As such, further research may be needed to properly determine the leakage rates (especially for seal leakage in the reactor vessel head), but not necessarily further modeling capabilities.

Vaporization and Noble Gas Decay Chains

The partitioning between sodium and vapor space of a few elements, as identified in Section 3.2.3, has been examined. For other elemental groups, such as americium, curium and plutonium, there is very little information related to solubility and evolution. With the substantial uncertainty associated with bypass, however, the need for further experimental work in this area is not indicated to be of high importance in the sensitivity studies. Sensitivity studies related to the impact of daughter products from the decay of noble gases were also conducted, and the results indicate that their contribution to the overall offsite consequence is negligible.

4 Conclusion

A trial MST calculation was performed, using available models and data, to identify gaps in current modeling capabilities and the associated database. In parallel, a sensitivity analysis was performed using a barrier-based fractional source term model to determine the importance of particular radionuclides and transport/retention phenomena in regard to offsite consequence. The primary finding of the study is that a SFR MST calculation is possible, with certain limitations, utilizing currently available tools and models. Gaps in models and data regarding some phenomena result in uncertainties, or the use of conservative assumptions, which could make the process of justifying reduced emergency planning zones or plant sites difficult for vendors and also potentially impact design decisions that are dependent on source term analyses.

Key Project Point

A SFR mechanistic source term calculation is possible, with certain limitations, utilizing currently available tools and models. Gaps in models and data regarding some phenomena result in uncertainties, or the use of conservative assumptions, which could make the process of justifying reduced emergency planning zones or plant sites difficult for vendors and also potentially impact design decisions that are dependent on source term analyses.

The findings of these two studies, in regards to gaps and importance, are reviewed in the following subsection, and a prioritization of gaps is established. This is followed by a subsection describing the practical issues encountered during the trial MST calculation process. The final subsection provides recommendations for future work, and possible gap closure pathways, based on the prioritization of gaps and practical issues encountered.

4.1 Prioritization of Gaps

The gaps identified during the trial MST calculation in Section 2 were grouped according to common radionuclide transport/retention mechanisms, as seen in Table 4-1. Each group was assigned an importance level based on the findings of the sensitivity calculation in Section 3 (with additional insights from the trial MST calculation).

A prioritization of the groups was established based on several factors, including: the gaps within the group, the impact of any associated assumptions (conservative/non-conservative), and the importance level from the sensitivity analysis. This ranking can be seen in Table 4-2. As the results show, the highest ranking gap was the assessment of bubble transport in the sodium pool. The phenomena related to this group represent a possible bypass mechanism of the sodium pool, which is a significant radionuclide barrier. There is very little validation data available to determine if the assumptions utilized for these phenomena are realistic. The importance of the gap is high, as the result of the calculation propagates through subsequent analysis steps, and it has a direct effect on the transport of non-noble gas radionuclides.

The next gap group relates to radionuclide migration within the fuel pin, and subsequent radionuclide release during fuel pin failure. As with the previous group, the assumptions in this portion of the analysis propagate through further analysis steps, and could result in potentially unrealistic releases (for example, the assumptions regarding transuranic migration and release resulted in surprisingly high quantities of these materials transporting to other regions of the reactor system).

Aerosol behavior is next, which includes the deposition/condensation of both aerosols and vapors, and possible chemical interactions. Although the importance of this mechanism was found to be lower than the

previous two groups in the sensitivity calculations, the impact of several of the analysis assumptions (especially those related to chemical interactions) are difficult to characterize as conservative or non-conservative. Also, while MELCOR will soon be able to model many of the phenomena within this group, sufficient data will be necessary to support the models.

Vaporization from the sodium pool was found to have low importance in the sensitivity calculation and trial MST calculation. However, if the impact of bubble transport is reduced, vaporization (and other pool release mechanisms) could become more important. It is difficult to characterize the assumptions used as conservative or non-conservative, as there is little quantitative data regarding many of the phenomena.

The “hold-up” of radionuclides within the cover gas region and containment is an important retention mechanism, and a detailed leakage analysis is currently difficult without a detailed design. However, applying conservative assumptions is straightforward, and the impact can be easily assessed (as shown in the trial MST calculation).

Lastly, offsite dispersion contains several key gaps related to the proper modeling of chemical and physical forms of radionuclides released from the plant. Although these gaps may have a direct impact on offsite consequence, the magnitude of their effect is likely below many of the gaps associated with radionuclide release fractions.

Table 4-1: Grouping of Gaps³¹

Group	Phenomena	Gap	Importance¹
<i>In-Pin Migration and Release</i>	<i>Radionuclide migration within the fuel pin during irradiation</i>	Partial	<i>H</i>
	<i>Radionuclide release fractions from failed fuel pins</i>	Partial	<i>H</i>
	<i>Radionuclide partitioning between gas and liquid/solid in plenum region</i>	Partial	<i>H</i>
	<i>Timing of radionuclide release from failed fuel pins</i>	Partial	<i>L</i>
<i>Bubble Transport</i>	<i>Partitioning of released radionuclides into bubbles or sodium pool</i>	Yes	<i>VH</i>
	<i>Bubble diameter</i>	Yes	<i>VH</i>
	<i>Aerosol particle size distribution</i>	Yes	<i>VH</i>
	<i>Aerosol particle density</i>	Partial	<i>VH</i>
	<i>Scrubbing of vapors/aerosols in bubble passing through sodium pool</i>	Partial	<i>VH</i>
<i>Vaporization</i>	<i>Vaporization from Sodium Pool (Thermodynamic Effects)</i>	Partial	<i>L</i>
	<i>Timing of Vaporization</i>	Yes	<i>L</i>
	<i>Kinetic Effects</i>	Yes	<i>L</i>
	<i>Non-homogenous Radionuclide Mixing (Surface-Boundary Concentration)</i>	Yes	<i>L</i>
	<i>Plate-out (Adsorption) and Settling in Sodium Pool</i>	Yes	<i>L</i>
	<i>Mechanical Forces (Liftoff due to Bubble Pop, Turbulence, or Convection)</i>	Yes	<i>L</i>
<i>Aerosol Behavior</i>	<i>Radionuclide Decay and Daughter Products</i>	Partial	<i>L</i>
	<i>Aerosol Agglomeration and Deposition</i>	Partial	<i>M</i>
	<i>Resuspension and Re-vaporization</i>	Yes	<i>M</i>
	<i>Aerosol Deposition in Flow Paths</i>	Yes	<i>M</i>
<i>Hold-up/Leakage</i>	<i>Cover Gas Temperature and Pressure Response</i>	Partial	<i>M</i>
	<i>Seal Leakage</i>	Yes	<i>M</i>
	<i>Containment Temperature and Pressure Response</i>	Yes	<i>M</i>
<i>Dispersion</i>	<i>Radionuclide Characteristics</i>	Partial	<i>L</i>
	<i>Chemical Interactions</i>	Yes	<i>L</i>
	<i>Dose Conversion Factors</i>	Partial	<i>L</i>

¹VH – Very High, H – High, M – Medium, L – Low

³¹ Those phenomena that were not associated with a gap, and those considered part of “accident modeling” rather than source term assessment, are not included in the table.

Table 4-2: Prioritization of Groups

Ranking	Group	Notes
1	Bubble Transport	<i>Represents a potential bypass mechanism of a major radionuclide barrier (the sodium pool). Very high importance in sensitivity calculations, and direct impact on non-noble gas radionuclide transport. Difficult to determine if analysis assumptions are realistic, and significant impact on subsequent analysis steps.</i>
2	In-Pin Migration and Release	<i>Determines initial radionuclide release fractions. High importance in sensitivity calculations. Conservative assumptions are straightforward to apply, but assumptions propagate through subsequent analysis steps, resulting in potentially unrealistic releases of transuranics.</i>
3	Aerosol Behavior	<i>Aerosol deposition/condensation is a significant retention mechanism, with medium importance in sensitivity calculations. Data regarding deposition, condensation, and chemical interactions are not as well-established as LWR data. Codes, such as MELCOR, have ability to model phenomena, but data are a necessary input.</i>
4	Hold-up/Leakage	<i>The delay in radionuclide releases due to hold-up in the cover gas region and containment. Medium importance in sensitivity calculations. Assumptions are straightforward to apply and characterize, as shown in trial MST calculation where multiple leakage values were assumed.</i>
5	Vaporization	<i>Vaporization of radionuclides from the sodium pool. Many gaps in the modeling of phenomena, but was low importance in sensitivity calculations (and in trial MST calculation). However, the relative importance of vaporization could increase, if bubble transport calculations can be shown to be overly conservative.</i>
6	Dispersion	<i>Radionuclide characteristics and dose conversion factors. Although these factors have a direct impact on offsite consequence, the magnitude of their influence is likely lower than the factors related to radionuclide release fractions from the plant.</i>

4.2 MST Analysis – Practical Issues Encountered

It is important to review practical issues encountered during the trial MST analysis before providing final recommendations for future work. There were a variety of difficulties or potential issues identified during the trial MST calculation that could make such an approach difficult to conduct.

Data Conversion

First, the analysis of radionuclide behavior within the fuel pin, and subsequent release to the sodium pool and cover gas region, utilized several computer codes (HSC, IFR bubble code, and ORIGEN) and other side calculations, which taken together, involved many data communication steps. Each transfer of information between codes presented an opportunity for error introduction as data was converted. For example, ORIGEN outputs isotopic masses. However, the chemistry code, HSC, utilizes elemental masses, as there are no changes in chemical properties for different isotopes of the same element. HSC would then output chemical forms, and fractional releases of elements to the cover gas region, which would then be converted back to isotopic mass. For the PLOF+ analysis, this conversion was repeated multiple times, as different fuel batches failed. The calculation process outlined in Figure 2-17 involved ten ORIGEN decay calculations, three HSC vaporization calculations, and three IFR bubble code calculations (not taking into account the ORIGEN and HSC calculations of radionuclide behavior within the fuel pin). Properly separating and combining data from the multiple analysis tools was not trivial, even for the simplified analysis of only three fuel batches. An attempt to perform a more precise source term assessment, with many different fuel groups within the core, would be a significant effort utilizing this framework.

Unfortunately, there is likely no direct resolution to the data transfer issue during the early phases of the MST analysis. Developing a single computer code that conducts radionuclide decay, thermodynamic equilibrium calculations, and radionuclide bubble transport seamlessly would be a significant effort. It is likely that resources could be better allocated addressing gaps in phenomena modeling, rather than the practical data transfer issues.

IFR Bubble Code

The bubble code utilized in the trial MST calculation was developed as part of the IFR project, which was terminated before the formal completion of the code. The original project plan was to develop the bubble transport code, then conduct a series of experiments to validate its performance, but the subsequent experimentation was not performed. Documentation regarding the code is currently considered Applied Technology, due to its association with the IFR project. For the bubble code to become available for use by U.S. SFR industry, the code must be formally completed, including the necessary documentation, and an avenue for establishing access and licensing must be formed. Additional detail regarding possible future work is provided in the following subsection.

CONTAIN-LMR

As described in Section 2.7 and Appendix A.4, many issues were encountered when attempting to utilize a developmental version of CONTAIN-LMR. These problems resulted in source code modifications and the necessary use of unrealistic assumptions, which prohibited the inclusion of the CONTAIN-LMR analysis within the current report. While a number of these issues have now been addressed, it would be very difficult for a vendor to utilize the code without the direct support of code developers. Fortunately, the transition of sodium-specific models from CONTAIN-LMR to MELCOR is currently underway, and while the new version of MELCOR was not yet available for inclusion in the current analysis, it is

important that code be finished promptly, as there is currently no U.S. supported SFR cover gas region and containment analysis code available.

Code Quality Assurance

It is important to note that with the exception of WinMACCS, all of the computer codes utilized during the trial MST analysis are research-oriented and have yet to be reviewed and endorsed by the NRC. For codes to be used in a licensing capacity, they must undergo a verification and validation process that meets the formal expectations of the NRC. The review process is different depending on whether the computer code will be used as an NRC confirmatory tool or a design tool by the licensing applicant. This consideration is also an important factor for the discussion of future research work, presented in the following subsection, as attention should be paid to licensing requirements during the planning of data and code quality assurance programs.

4.3 Recommendations for Future Research

Based on the findings of the trial MST calculation and the sensitivity analysis, several avenues for future research were explored, as shown in Table 4-3. The remainder of this section provides additional detail on each future research pathway.

Table 4-3: Recommendations for Future Research

Group	Recommendations
<i>Bubble Transport</i>	<ul style="list-style-type: none"> • Formal completion of the IFR bubble code, including development of documentation and code licensing pathway. • Experimentation regarding failed fuel pin blowdown and entrainment of released radionuclides in bubble (cross-cutting research with reactivity effects of channel voiding and structural impacts of blowdown on neighboring fuel pins). • Experimentation regarding removal of radionuclides from bubble traveling through sodium pool.
<i>In-Pin Migration and Release</i>	<ul style="list-style-type: none"> • Continued metal fuel PIE to determine radionuclide migration within fuel pin during irradiation. • Experimentation regarding radionuclide release from failed high burnup fuel pins at high temperatures (above fuel melting point) in liquid sodium.
<i>Aerosol Behavior</i>	<ul style="list-style-type: none"> • Continued development of SFR version of MELCOR. • Assessment of available data regarding deposition/condensation/chemical interactions within cover gas region and containment.
<i>Hold-up/Leakage</i>	<ul style="list-style-type: none"> • Response of reactor head seals during transient conditions.
<i>Vaporization</i>	<ul style="list-style-type: none"> • Investigation of non-homogeneous mixing of radionuclides in liquid sodium.
<i>Dispersion</i>	<ul style="list-style-type: none"> • Assessment of applicability of dose conversion factors and deposition assumptions to chemical and physical radionuclide forms likely in SFR radionuclide release.

Bubble Transport

Perhaps the clearest potential research area relates to bubble transport phenomena. This area considers two separate issues. First, the IFR bubble code must be formally completed, and an avenue for industry access must be established, as described in the preceding subsection. Second, there are significant uncertainties regarding the formation of bubbles after the failure of the fuel pins, including what radionuclides become entrained within bubbles (and their aerosol size) and the behavior of bubbles as they transport through the sodium pool. There is very little experimental data available to justify the assumptions utilized in this part of the MST analysis. Fortunately, many of the gaps could be addressed through experimentation with non-radioactive elements, as bubble behavior and elemental chemistry are not isotope-dependent.

As shown in Figure 4-1, the research needed to provide information for gap closure could be divided into separate experiments. First, simulated pin-blowdown tests could be performed to examine the formation of bubbles in the coolant channels, and explore the dispersal of elements and bond sodium within the bubbles. These tests would also have cross-over application to research areas regarding the possible reactivity effects of sodium voiding due to fuel pin failures, and the structure impact of fuel pin failures on neighboring fuel pins and structure (for example, could the failure of a high burnup, high internal pressure fuel pin result in the failure of neighboring fuel pins).

The second area of experimentation involves the examination of bubble transport within the sodium pool. The focus of these tests would be the behavior of the bubble as it passes through the pool (including possible impacts with structure), and the removal of aerosols and vapors within the bubble. Again, non-radioactive isotopes of the elements of interest could be used. For both experimental areas, it may be possible to find a suitable surrogate fluid, that is less reactive than sodium, and possibly transparent, to aid in characterizing phenomena. However, even if sodium experiments are necessary, there are multiple U.S. facilities available that could perform such work.

Figure 4-1: Distinction of Bubble Transport Experimentation

In-pin Migration and Release

Many of the gaps related to radionuclide migration within the fuel pin during irradiation, and subsequent release during fuel pin failure, have already been discussed in detail in ANL-ART-38. However, an overview is provided here for completeness. The first gap relates to insufficient post-irradiation examination (PIE) data regarding the migration of radionuclides during fuel irradiation. The limitations of available data result in, what are likely, overly conservative estimates of the migration of transuranics to the bond sodium, which are later assumed to be released from the fuel pin after cladding failure. The second gap pertains to the release of radionuclides from molten fuel in liquid sodium. Very little experimentation exists in this area, and it is difficult to characterize the current assumptions as conservative or optimistic.

The second gap, relating to the release of radionuclides from molten fuel into liquid sodium, is particularly challenging. However, the restart of the TREAT facility in Idaho may present a unique opportunity. As discussed in Section 2.2.3, metal fuel pins were subjected to transient overpower in the TREAT facility, while immersed in flowing sodium. The severity of the transient overpower resulted in fuel melting and the failure of fuel pins. Unfortunately, at the time, the test loops were not equipped to assess radionuclide release from the failed fuel. With the TREAT restart, it may be possible to perform similar experiments utilizing metal fuel (MFF series) from FFTF. The MFF series fuel represents the most prototypic metal fuel in the U.S. An experiment utilizing the MFF series fuel in flowing liquid sodium in the TREAT facility would provide valuable data, as experimental fuel failure conditions would be directly applicable to potential reactor fuel failure transients.

Aerosol Behavior

The most beneficial research to be conducted regarding aerosol behavior is the continued development of the SFR version of MELCOR. With the difficulties experienced when attempting to utilize the developmental version of CONTAIN-LMR, it is imperative that a supported, stable code is available for the analysis of radionuclide behavior in the cover gas region and containment. In addition, a detailed assessment of the applicability of available data regarding the assessment of SFR-specific aerosols and chemical forms would aid in the determination of needs regarding experimentation in this area. Similar studies have been performed in the past, and provide a useful starting point for additional analysis [4, 53, 54].

Hold-up/Leakage

A major uncertainty in the trial MST calculation was the response of the reactor head seals to the temperature and pressure conditions experienced during the transient scenarios. Although seal testing has been performed in the past³², there is little data regarding the performance of the seals at very high temperatures or pressures. In particular, the degree of seal leakage at above-nominal temperatures and pressure, and the ability to reseal once temperatures and pressures are reduced (as opposed to failure, where leakage still occurs even after conditions return to nominal) are of specific interest and such data could be used to develop realistic models.

Vaporization

Radionuclide vaporization from the sodium pool was considered to be of low importance when compared to the possibility of radionuclide transport within bubbles. However, the impact of vaporization could increase if non-homogeneous mixing of radionuclides occurs within the sodium pool. This possibility has been seen in some past experimentation (see Section 4.2 of ref [5]). A relatively small series of experiments, utilizing non-radioactive elemental forms, could provide definitive data regarding this phenomenon. Based on the results, this issue could be completely resolved and likely removed from future licensing concerns, or if shown to be of significant impact, updated models could be developed from the results.

Dispersion

There are two main areas that could use additional research in the area of offsite dispersion. First, a comparison of radionuclide chemical and physical forms following releases from SFRs and LWRs would provide an indication of the applicability of LWR deposition factors for SFR offsite dispersion analyses. Second, a study regarding the applicability of dose conversion factors typically utilized for LWR assessments to SFR radionuclide forms would assist in reducing the uncertainty regarding this effect.

³² A major seal test program was conducted from 1973-1979 as part of FFTF development, see ref [55] (and many subsequent progress reports) for details.

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Regulatory Technology Development Plan

Sodium Fast Reactor

Mechanistic Source Term – Trial Calculation

Nuclear Engineering Division

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Regulatory Technology Development Plan

Sodium Fast Reactor

Mechanistic Source Term – Trial Calculation

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Appendix A: Mechanistic Source Term Trial Calculation Details

The following subsections provide additional calculation details for each of the trial MST analysis steps.

A.1 Fuel Batch Radionuclide Inventory

This section provides the fuel pin inventory for the three fuel batches of the reference reactor. Table A - 1 contains the fuel pin inventory at time zero, while Table A - 2 provides the fuel pin inventory for the PLOF+ at the time of fuel pin failure, which has undergone a period of radioactive decay.

Table A - 1: Fuel Batch Pin Radionuclide Inventory at Time = 0

Inventory Per Pin (g)											
Isotope	Batch A	Batch B	Batch C	Isotope	Batch A	Batch B	Batch C	Isotope	Batch A	Batch B	Batch C
i121	1.11E-18	1.25E-18	1.25E-18	am242m	1.64E-01	1.67E-01	1.61E-01	ce143	1.09E-03	1.10E-03	1.10E-03
i123	8.48E-15	8.43E-15	8.39E-15	am243	1.08E+00	1.08E+00	1.08E+00	ce144	1.10E-01	1.70E-01	1.91E-01
i124	7.32E-18	7.72E-18	8.24E-18	am244	1.38E-05	1.45E-05	1.50E-05	ce145	1.19E-06	1.19E-06	1.19E-06
i125	2.16E-13	9.72E-13	2.16E-12	am244m	8.26E-06	8.64E-06	8.98E-06	ce146	4.46E-06	4.45E-06	4.45E-06
i126	9.46E-09	2.61E-08	4.31E-08	am245	1.77E-10	4.61E-10	7.63E-10	ce147	2.41E-07	2.41E-07	2.41E-07
i127	1.42E-02	3.62E-02	5.71E-02	am246	1.37E-14	1.44E-14	1.51E-14	ce148	1.60E-07	1.61E-07	1.61E-07
i128	4.00E-08	1.06E-07	1.74E-07	am246m	8.13E-15	8.53E-15	8.96E-15	ce149	9.42E-09	9.43E-09	9.44E-09
i129	4.55E-02	1.13E-01	1.79E-01	am247	4.53E-16	1.03E-15	1.52E-15	ce150	3.82E-09	3.83E-09	3.84E-09
i130	2.30E-06	5.61E-06	9.05E-06	ba129	0.00E+00	0.00E+00	0.00E+00	ce151	5.57E-10	5.60E-10	5.62E-10
i130m	1.68E-08	4.23E-08	6.88E-08	ba131	4.21E-15	3.21E-14	8.37E-14	ce152	1.29E-10	1.30E-10	1.31E-10
i131	4.78E-03	4.77E-03	4.76E-03	ba132	2.84E-08	1.96E-07	4.87E-07	ce153	1.96E-11	1.98E-11	1.99E-11
i132	8.19E-05	8.17E-05	8.16E-05	ba133	7.46E-10	2.56E-08	1.22E-07	ce154	2.02E-12	2.03E-12	2.04E-12
i132m	8.60E-07	8.55E-07	8.51E-07	ba134	3.39E-04	5.43E-03	1.84E-02	ce155	1.19E-13	1.20E-13	1.20E-13
i133	9.83E-04	9.81E-04	9.79E-04	ba135	1.57E-06	5.60E-05	2.81E-04	ce156	5.85E-15	5.88E-15	5.90E-15
i133m	1.29E-08	1.28E-08	1.28E-08	ba135m	3.00E-09	3.33E-08	1.13E-07	ce157	1.53E-16	1.53E-16	1.54E-16
i134	4.48E-05	4.48E-05	4.47E-05	ba136	4.67E-03	1.97E-02	4.29E-02	cm240	4.87E-11	6.24E-11	6.13E-11
i134m	3.98E-07	3.96E-07	3.94E-07	ba136m	1.03E-11	2.07E-11	3.17E-11	cm241	1.19E-08	1.54E-08	1.52E-08
i135	3.00E-04	3.00E-04	2.99E-04	ba137	2.79E-03	1.72E-02	4.15E-02	cm242	9.71E-02	1.13E-01	1.05E-01
i136	4.14E-07	4.14E-07	4.15E-07	ba137m	3.93E-08	9.51E-08	1.49E-07	cm243	5.21E-03	6.05E-03	6.63E-03
i136m	1.51E-07	1.50E-07	1.50E-07	ba138	2.41E-01	6.04E-01	9.65E-01	cm244	5.46E-01	6.08E-01	6.64E-01
i137	1.36E-07	1.36E-07	1.36E-07	ba139	5.74E-05	5.73E-05	5.72E-05	cm245	1.16E-01	1.17E-01	1.21E-01
i138	1.93E-08	1.93E-08	1.93E-08	ba140	1.21E-02	1.21E-02	1.21E-02	cm246	6.63E-02	6.68E-02	6.74E-02
i139	2.58E-09	2.59E-09	2.59E-09	ba141	1.15E-05	1.14E-05	1.14E-05	cm247	2.08E-03	4.53E-03	6.44E-03
i140	2.83E-10	2.84E-10	2.85E-10	ba142	6.03E-06	6.02E-06	6.01E-06	cm248	2.40E-05	1.42E-04	3.25E-04
i141	3.29E-11	3.30E-11	3.31E-11	ba143	1.13E-07	1.13E-07	1.13E-07	cm249	8.36E-11	5.18E-10	1.23E-09
i142	3.06E-12	3.07E-12	3.08E-12	ba144	6.41E-08	6.41E-08	6.41E-08	cm250	6.17E-13	1.06E-11	3.81E-11
i143	5.21E-13	5.23E-13	5.25E-13	ba145	1.11E-08	1.12E-08	1.12E-08	cm251	4.28E-19	7.69E-18	2.86E-17
i144	5.44E-15	5.47E-15	5.49E-15	ba146	2.51E-09	2.52E-09	2.53E-09	co 65	4.89E-18	4.91E-18	4.93E-18
u230	6.40E-15	3.35E-14	7.35E-14	ba147	2.94E-10	2.95E-10	2.97E-10	co 66	2.61E-16	2.62E-16	2.63E-16
u231	8.58E-13	3.22E-12	5.94E-12	ba148	4.77E-11	4.80E-11	4.82E-11	co 67	1.51E-15	1.52E-15	1.52E-15
u232	6.00E-07	2.12E-06	3.76E-06	ba149	4.50E-12	4.52E-12	4.54E-12	co 68	8.74E-16	8.78E-16	8.80E-16
u233	9.37E-06	1.93E-05	2.60E-05	ba150	4.30E-13	4.32E-13	4.33E-13	co 69	9.63E-16	9.67E-16	9.69E-16
u234	4.62E-01	4.34E-01	4.07E-01	ba151	6.09E-14	6.11E-14	6.13E-14	co 70	3.72E-16	3.73E-16	3.74E-16
u235	1.57E-01	1.39E-01	1.23E-01	ba152	8.71E-16	8.75E-16	8.78E-16	co 71	1.26E-16	1.27E-16	1.27E-16
u235m	6.01E-07	5.88E-07	5.74E-07	ba153	2.88E-17	2.89E-17	2.90E-17	co 72	3.38E-17	3.39E-17	3.39E-17
u236	2.41E-01	2.38E-01	2.34E-01	br 75	3.89E-25	3.23E-24	1.09E-23	co 73	8.42E-18	8.45E-18	8.47E-18
u237	1.19E-03	1.20E-03	1.21E-03	br 77	4.94E-15	4.96E-15	4.94E-15	co 74	9.78E-19	9.82E-19	9.85E-19
u238	2.15E+02	2.07E+02	2.00E+02	br 77m	4.80E-18	4.81E-18	4.80E-18	co 75	1.54E-19	1.55E-19	1.56E-19
u239	3.02E-04	3.03E-04	3.04E-04	br 78	9.14E-16	9.39E-16	9.63E-16	cs127	3.76E-25	1.32E-23	5.74E-23
u240	7.09E-16	1.77E-15	2.82E-15	br 79	5.23E-07	1.27E-06	1.98E-06	cs129	1.63E-17	1.96E-17	1.96E-17
u241	5.11E-19	1.33E-18	2.21E-18	br 79m	6.45E-16	6.41E-16	6.37E-16	cs131	4.09E-12	4.88E-12	5.60E-12
y 90	1.45E-05	3.58E-05	5.65E-05	br 80	3.65E-12	6.35E-12	9.13E-12	cs132	9.23E-08	2.43E-07	3.98E-07
y 90m	1.48E-09	2.60E-09	3.79E-09	br 80m	3.16E-11	4.67E-11	6.23E-11	cs133	2.50E-01	6.21E-01	9.77E-01
y 91	1.68E-02	1.71E-02	1.71E-02	br 81	3.40E-03	8.33E-03	1.31E-02	cs134	3.37E-03	1.93E-02	4.28E-02
y 91m	5.97E-06	5.96E-06	5.95E-06	br 82	6.17E-07	1.36E-06	2.14E-06	cs134m	3.85E-07	9.91E-07	1.62E-06
y 92	5.23E-05	5.21E-05	5.20E-05	br 82m	1.40E-09	3.41E-09	5.49E-09	cs135	2.82E-01	7.00E-01	1.11E+00
y 93	1.88E-04	1.87E-04	1.87E-04	br 83	3.12E-06	3.12E-06	3.11E-06	cs135m	2.85E-08	2.87E-08	2.91E-08
y 93m	1.45E-09	1.45E-09	1.45E-09	br 84	1.11E-06	1.11E-06	1.11E-06	cs136	3.40E-04	6.86E-04	1.05E-03
y 94	6.37E-06	6.35E-06	6.33E-06	br 84m	1.50E-08	1.49E-08	1.48E-08	cs136m	1.56E-09	1.65E-09	1.75E-09
y 95	3.90E-06	3.88E-06	3.88E-06	br 85	1.20E-07	1.20E-07	1.20E-07	cs137	2.51E-01	6.16E-01	9.70E-01
y 96	1.95E-08	1.94E-08	1.94E-08	br 86	5.05E-08	5.04E-08	5.02E-08	cs138	2.40E-05	2.40E-05	2.40E-05
y 96m	2.54E-08	2.53E-08	2.52E-08	br 87	5.67E-08	5.66E-08	5.65E-08	cs138m	1.70E-07	1.69E-07	1.69E-07
y 97	1.27E-08	1.27E-08	1.27E-08	br 88	1.34E-08	1.34E-08	1.34E-08	cs139	6.20E-06	6.19E-06	6.18E-06
y 97m	2.63E-09	2.63E-09	2.62E-09	br 89	3.11E-09	3.11E-09	3.11E-09	cs140	5.74E-07	5.74E-07	5.73E-07
y 98	1.40E-09	1.40E-09	1.40E-09	br 90	8.50E-10	8.51E-10	8.51E-10	cs141	1.83E-07	1.83E-07	1.83E-07
y 98m	3.45E-09	3.45E-09	3.44E-09	br 91	8.48E-11	8.51E-11	8.53E-11	cs142	6.82E-09	6.83E-09	6.83E-09
y 99	4.07E-09	4.07E-09	4.07E-09	br 92	1.46E-11	1.46E-11	1.47E-11	cs143	3.81E-09	3.82E-09	3.82E-09
y100	8.53E-10	8.56E-10	8.57E-10	br 93	1.32E-12	1.32E-12	1.32E-12	cs144	8.24E-10	8.28E-10	8.30E-10
y101	1.92E-10	1.93E-10	1.93E-10	br 94	2.15E-13	2.15E-13	2.14E-13	cs145	1.24E-10	1.24E-10	1.25E-10
y102	4.17E-11	4.19E-11	4.21E-11	br 95	1.53E-15	1.53E-15	1.54E-15	cs146	1.18E-11	1.19E-11	1.19E-11
y103	5.99E-12	6.01E-12	6.04E-12	br 96	2.58E-16	2.59E-16	2.60E-16	cs147	1.09E-12	1.09E-12	1.10E-12
y104	5.53E-13	5.55E-13	5.57E-13	br 97	6.73E-18	6.73E-18	6.73E-18	cs148	9.04E-14	9.08E-14	9.12E-14
y105	5.46E-14	5.48E-14	5.50E-14	ce135	1.30E-18	1.57E-18	1.53E-18	cs149	5.85E-16	5.88E-16	5.90E-16
y106	1.11E-16	1.12E-16	1.13E-16	ce137	1.20E-14	1.36E-14	1.35E-14	cs150	5.96E-17	5.99E-17	6.01E-17
y107	7.20E-18	7.23E-18	7.25E-18	ce138	3.55E-10	1.13E-09	2.07E-09	cs151	1.04E-17	1.04E-17	1.05E-17
y108	4.73E-20	4.75E-20	4.76E-20	ce139	8.30E-07	3.41E-06	6.35E-06	eu147	2.34E-17	2.97E-17	2.91E-17
am239	2.25E-12	2.03E-12	1.83E-12	ce139m	2.39E-12	6.44E-12	1.08E-11	eu149	2.16E-13	3.39E-13	3.46E-13
am240	2.14E-07	1.93E-07	1.74E-07	ce140	2.14E-01	5.55E-01	8.97E-01	eu151	1.02E-04	5.30E-04	1.09E-03
am241	2.12E+00	1.84E+00	1.59E+00	ce141	2.96E-02	2.96E-02	2.96E-02	eu152	5.44E-06	7.05E-05	2.09E-04
am242	6.31E-04	5.68E-04	5.13E-04	ce142	1.96E-01	4.90E-01	7.82E-01	eu152m	1.52E-08	8.20E-08	1.75E-07

Table A - 1: Fuel Batch Pin Radionuclide Inventory at Time = 0 (cont.)

Isotope	Batch A	Batch B	Batch C	Isotope	Batch A	Batch B	Batch C	Isotope	Batch A	Batch B	Batch C
eu153	1.72E-02	4.03E-02	6.11E-02	mo 99	2.08E-03	2.09E-03	2.11E-03	nd161	4.04E-16	4.08E-16	4.10E-16
eu154	1.29E-03	7.22E-03	1.58E-02	mo100	1.88E-01	4.67E-01	7.44E-01	np234	1.85E-15	3.87E-15	5.35E-15
eu154m	6.67E-09	1.62E-08	2.54E-08	mo101	7.92E-06	7.98E-06	8.04E-06	np235	4.85E-09	8.27E-09	9.90E-09
eu155	7.87E-03	1.81E-02	2.78E-02	mo102	6.25E-06	6.25E-06	6.23E-06	np236	2.02E-06	4.25E-06	5.84E-06
eu156	4.40E-04	4.94E-04	5.49E-04	mo103	6.57E-07	6.56E-07	6.55E-07	np236m	3.47E-08	3.54E-08	3.60E-08
eu157	1.11E-05	1.11E-05	1.11E-05	mo104	5.11E-07	5.10E-07	5.10E-07	np237	3.33E-01	3.26E-01	3.18E-01
eu158	3.38E-07	3.39E-07	3.40E-07	mo105	2.23E-07	2.23E-07	2.23E-07	np238	3.41E-04	3.48E-04	3.53E-04
eu159	7.06E-08	7.08E-08	7.10E-08	mo106	3.31E-08	3.31E-08	3.31E-08	np239	4.36E-02	4.38E-02	4.39E-02
eu160	1.14E-09	1.15E-09	1.15E-09	mo107	4.84E-09	4.86E-09	4.87E-09	np240	4.07E-07	4.25E-07	4.44E-07
eu161	3.43E-10	3.45E-10	3.47E-10	mo108	4.96E-10	4.98E-10	4.99E-10	np240m	7.88E-08	8.24E-08	8.61E-08
eu162	4.23E-11	4.26E-11	4.29E-11	mo109	3.08E-11	3.11E-11	3.13E-11	np241	9.00E-13	9.25E-13	9.46E-13
eu163	8.06E-12	8.13E-12	8.22E-12	mo110	3.69E-12	3.71E-12	3.72E-12	pd 99	0.00E+00	0.00E+00	0.00E+00
eu164	5.48E-13	5.54E-13	5.60E-13	mo111	6.75E-13	6.78E-13	6.80E-13	pd101	7.63E-17	1.27E-15	4.12E-15
eu165	8.10E-14	8.17E-14	8.25E-14	mo112	1.37E-13	1.37E-13	1.38E-13	pd102	1.96E-08	3.12E-07	9.77E-07
eu166	2.20E-15	2.22E-15	2.23E-15	mo113	5.64E-15	5.66E-15	5.68E-15	pd103	1.92E-09	1.81E-08	4.96E-08
eu167	1.72E-16	1.73E-16	1.73E-16	mo114	2.87E-16	2.88E-16	2.88E-16	pd104	2.98E-03	2.39E-02	6.17E-02
kr 77	2.08E-26	5.70E-25	2.43E-24	mo115	2.25E-17	2.26E-17	2.27E-17	pd105	1.57E-01	3.78E-01	5.83E-01
kr 78	8.30E-17	3.04E-16	5.30E-16	nb 89	1.20E-20	1.45E-20	1.41E-20	pd106	3.80E-02	1.92E-01	4.00E-01
kr 79	2.00E-15	2.91E-15	4.29E-15	nb 90	1.05E-17	1.27E-17	1.24E-17	pd107	9.81E-02	2.35E-01	3.62E-01
kr 79m	3.96E-19	5.79E-19	8.58E-19	nb 90m	3.58E-25	9.86E-25	1.66E-24	pd107m	2.72E-11	1.42E-10	3.05E-10
kr 80	4.68E-08	1.76E-07	3.64E-07	nb 91	1.41E-12	3.72E-12	6.02E-12	pd108	7.13E-02	1.90E-01	3.19E-01
kr 81	3.27E-09	1.05E-08	2.17E-08	nb 91m	2.16E-17	6.95E-17	1.21E-16	pd109	1.15E-04	1.20E-04	1.25E-04
kr 81m	4.44E-16	1.02E-15	1.93E-15	nb 92	1.20E-10	3.06E-10	4.89E-10	pd109m	4.66E-10	1.13E-09	1.89E-09
kr 82	5.90E-05	3.02E-04	7.04E-04	nb 92m	9.35E-15	5.54E-14	1.35E-13	pd110	2.37E-02	5.89E-02	9.95E-02
kr 83	7.07E-03	1.74E-02	2.75E-02	nb 93	7.82E-09	2.53E-08	5.17E-08	pd111	8.48E-07	8.69E-07	8.90E-07
kr 83m	2.38E-06	2.38E-06	2.37E-06	nb 93m	2.12E-08	1.28E-07	3.03E-07	pd111m	8.78E-08	1.32E-07	1.78E-07
kr 84	1.24E-02	3.11E-02	4.99E-02	nb 94	5.72E-07	1.75E-06	2.94E-06	pd112	2.27E-05	2.28E-05	2.30E-05
kr 85	3.04E-03	7.27E-03	1.12E-02	nb 94m	9.10E-12	9.89E-12	1.03E-11	pd113	1.81E-08	1.82E-08	1.83E-08
kr 85m	1.12E-05	1.12E-05	1.12E-05	nb 95	1.82E-02	1.93E-02	1.94E-02	pd114	1.94E-08	1.94E-08	1.95E-08
kr 86	2.00E-02	4.99E-02	7.98E-02	nb 95m	2.11E-05	2.17E-05	2.17E-05	pd115	2.54E-09	2.55E-09	2.55E-09
kr 87	6.02E-06	6.00E-06	5.99E-06	nb 96	2.55E-06	2.78E-06	2.88E-06	pd116	1.02E-09	1.02E-09	1.02E-09
kr 88	1.71E-05	1.71E-05	1.71E-05	nb 97	3.22E-05	3.22E-05	3.22E-05	pd117	2.52E-10	2.52E-10	2.52E-10
kr 89	3.81E-07	3.80E-07	3.79E-07	nb 97m	4.13E-07	4.13E-07	4.13E-07	pd118	6.64E-11	6.66E-11	6.67E-11
kr 90	6.45E-08	6.43E-08	6.42E-08	nb 98	2.28E-08	2.28E-08	2.27E-08	pd119	1.31E-11	1.32E-11	1.32E-11
kr 91	1.28E-08	1.28E-08	1.28E-08	nb 98m	1.42E-07	1.42E-07	1.41E-07	pd120	2.85E-12	2.87E-12	2.88E-12
kr 92	1.72E-09	1.72E-09	1.72E-09	nb 99	7.60E-08	7.59E-08	7.57E-08	pd121	5.11E-13	5.13E-13	5.15E-13
kr 93	4.83E-10	4.85E-10	4.86E-10	nb 99m	5.51E-07	5.49E-07	5.48E-07	pd122	8.72E-14	8.75E-14	8.78E-14
kr 94	3.24E-11	3.25E-11	3.26E-11	nb100	1.27E-08	1.27E-08	1.27E-08	pd123	2.60E-14	2.61E-14	2.62E-14
kr 95	2.76E-12	2.77E-12	2.78E-12	nb100m	2.77E-09	2.76E-09	2.75E-09	pd124	6.61E-16	6.64E-16	6.66E-16
kr 96	9.16E-13	9.13E-13	9.11E-13	nb101	6.16E-08	6.15E-08	6.14E-08	pm141	0.00E+00	0.00E+00	0.00E+00
kr 97	7.99E-14	7.94E-14	7.90E-14	nb102	2.12E-08	2.12E-08	2.12E-08	pm143	7.61E-15	1.78E-14	2.14E-14
kr 98	2.28E-15	2.26E-15	2.25E-15	nb102m	2.92E-09	2.92E-09	2.91E-09	pm144	4.39E-13	1.13E-12	1.63E-12
kr 99	9.87E-17	9.91E-17	9.94E-17	nb103	7.99E-09	7.99E-09	7.99E-09	pm145	2.05E-10	2.80E-09	8.96E-09
kr100	4.62E-19	4.62E-19	4.61E-19	nb104	7.39E-09	7.41E-09	7.42E-09	pm146	2.46E-06	1.33E-05	2.75E-05
la133	4.44E-19	5.36E-19	5.25E-19	nb104m	1.13E-09	1.14E-09	1.14E-09	pm147	7.30E-02	1.50E-01	2.01E-01
la135	7.35E-14	8.02E-14	7.99E-14	nb105	3.43E-09	3.44E-09	3.45E-09	pm148	7.71E-05	1.69E-04	2.35E-04
la137	8.28E-08	2.11E-07	3.37E-07	nb106	2.32E-10	2.34E-10	2.35E-10	pm148m	4.12E-04	1.00E-03	1.43E-03
la138	4.93E-06	2.50E-05	5.82E-05	nb107	1.65E-11	1.66E-11	1.66E-11	pm149	5.52E-04	5.64E-04	5.76E-04
la139	2.27E-01	5.65E-01	9.03E-01	nb108	1.20E-12	1.21E-12	1.22E-12	pm150	6.36E-08	6.62E-08	6.88E-08
la140	1.65E-03	1.65E-03	1.65E-03	nb109	9.25E-14	9.30E-14	9.33E-14	pm151	1.79E-04	1.82E-04	1.86E-04
la141	1.49E-04	1.49E-04	1.49E-04	nb110	6.45E-15	6.47E-15	6.49E-15	pm152	3.21E-07	3.20E-07	3.20E-07
la142	5.43E-05	5.42E-05	5.41E-05	nb111	4.26E-15	4.28E-15	4.29E-15	pm152m	1.84E-08	1.84E-08	1.83E-08
la143	7.79E-06	7.78E-06	7.77E-06	nb112	3.74E-17	3.76E-17	3.77E-17	pm153	2.90E-07	2.91E-07	2.91E-07
la144	3.23E-07	3.22E-07	3.22E-07	nb113	2.97E-18	2.98E-18	2.99E-18	pm154	5.35E-08	5.36E-08	5.36E-08
la145	1.44E-07	1.43E-07	1.43E-07	nd140	2.93E-17	3.89E-17	4.50E-17	pm154m	1.44E-08	1.43E-08	1.43E-08
la146	1.52E-08	1.52E-08	1.52E-08	nd141	1.95E-12	1.62E-11	4.37E-11	pm155	1.61E-08	1.61E-08	1.61E-08
la146m	1.29E-08	1.29E-08	1.29E-08	nd141m	2.62E-15	2.17E-14	5.87E-14	pm156	5.75E-09	5.76E-09	5.76E-09
la147	8.24E-09	8.26E-09	8.27E-09	nd142	5.78E-04	4.57E-03	1.19E-02	pm157	1.04E-09	1.04E-09	1.04E-09
la148	9.50E-10	9.55E-10	9.59E-10	nd143	1.68E-01	4.32E-01	6.90E-01	pm158	1.44E-10	1.45E-10	1.46E-10
la149	3.16E-10	3.18E-10	3.19E-10	nd144	5.13E-02	2.38E-01	4.68E-01	pm159	1.08E-11	1.09E-11	1.09E-11
la150	6.59E-11	6.63E-11	6.66E-11	nd145	1.28E-01	3.13E-01	4.92E-01	pm160	1.77E-12	1.79E-12	1.81E-12
la151	1.08E-11	1.08E-11	1.09E-11	nd146	1.11E-01	2.82E-01	4.60E-01	pm161	1.47E-13	1.49E-13	1.50E-13
la152	7.55E-13	7.59E-13	7.63E-13	nd147	4.30E-03	4.36E-03	4.41E-03	pm162	2.06E-15	2.07E-15	2.08E-15
la153	5.93E-14	5.96E-14	5.98E-14	nd148	7.35E-02	1.82E-01	2.90E-01	pm163	1.14E-16	1.15E-16	1.15E-16
la154	1.70E-15	1.71E-15	1.72E-15	nd149	1.75E-05	1.83E-05	1.86E-05	pr139	8.10E-16	9.55E-16	9.39E-16
la155	4.08E-17	4.10E-17	4.11E-17	nd150	4.46E-02	1.10E-01	1.75E-01	pr140	1.93E-11	5.49E-11	9.28E-11
mo 90	0.00E+00	0.00E+00	0.00E+00	nd151	1.29E-06	1.32E-06	1.34E-06	pr141	1.78E-01	4.86E-01	7.90E-01
mo 91	3.92E-22	4.73E-22	4.61E-22	nd152	8.73E-07	8.73E-07	8.72E-07	pr142	4.58E-06	1.31E-05	2.20E-05
mo 92	6.53E-16	2.84E-15	6.82E-15	nd153	2.48E-08	2.49E-08	2.49E-08	pr142m	2.04E-08	5.80E-08	9.80E-08
mo 93	1.11E-12	3.30E-11	1.42E-10	nd154	1.10E-08	1.11E-08	1.11E-08	pr143	1.04E-02	1.04E-02	1.04E-02
mo 93m	1.71E-16	2.15E-16	2.81E-16	nd155	1.59E-09	1.60E-09	1.60E-09	pr144	4.64E-06	7.18E-06	8.06E-06
mo 94	1.24E-06	1.41E-05	3.95E-05	nd156	3.51E-10	3.53E-10	3.54E-10	pr144m	2.23E-08	3.25E-08	3.61E-08
mo 95	7.30E-02	2.55E-01	4.33E-01	nd157	2.82E-11	2.84E-11	2.86E-11	pr145	1.42E-04	1.42E-04	1.42E-04
mo 96	9.23E-04	7.27E-03	1.89E-02	nd158	3.32E-12	3.36E-12	3.39E-12	pr146	8.02E-06	8.02E-06	8.00E-06
mo 97	1.45E-01	3.57E-01	5.64E-01	nd159	1.99E-13	2.01E-13	2.03E-13	pr147	3.62E-06	3.62E-06	3.61E-06
mo 98	1.59E-01	4.01E-01	6.46E-01	nd160	1.11E-14	1.12E-14	1.13E-14	pr148	4.52E-07	4.52E-07	4.52E-07

Table A - 1: Fuel Batch Pin Radionuclide Inventory at Time = 0 (cont.)

Isotope	Batch A	Batch B	Batch C	Isotope	Batch A	Batch B	Batch C	Isotope	Batch A	Batch B	Batch C
pr148m	5.13E-08	5.10E-08	5.07E-08	rh118	8.28E-13	8.32E-13	8.35E-13	se 79m	1.13E-08	1.12E-08	1.12E-08
pr149	3.74E-07	3.74E-07	3.74E-07	rh119	1.25E-13	1.26E-13	1.26E-13	se 80	1.84E-03	4.58E-03	7.32E-03
pr150	1.22E-08	1.22E-08	1.22E-08	rh120	2.05E-14	2.05E-14	2.06E-14	se 81	1.93E-07	1.92E-07	1.92E-07
pr151	2.21E-08	2.21E-08	2.22E-08	rh121	3.66E-15	3.68E-15	3.69E-15	se 81m	7.26E-08	7.24E-08	7.22E-08
pr152	2.02E-09	2.02E-09	2.03E-09	rh122	3.28E-16	3.30E-16	3.31E-16	se 82	4.94E-03	1.23E-02	1.97E-02
pr153	9.83E-10	9.88E-10	9.92E-10	ru 95	1.62E-31	7.32E-31	1.58E-30	se 83	4.22E-07	4.21E-07	4.20E-07
pr154	1.37E-10	1.38E-10	1.38E-10	ru 96	3.54E-22	1.54E-21	3.19E-21	se 83m	2.31E-09	2.31E-09	2.31E-09
pr155	1.24E-11	1.25E-11	1.25E-11	ru 97	5.23E-17	8.11E-17	1.16E-16	se 84	1.10E-07	1.09E-07	1.09E-07
pr156	1.63E-12	1.65E-12	1.66E-12	ru 98	6.63E-11	4.62E-10	1.20E-09	se 85	1.67E-08	1.66E-08	1.66E-08
pr157	1.59E-13	1.60E-13	1.61E-13	ru 99	5.63E-06	1.49E-05	2.50E-05	se 86	7.29E-09	7.28E-09	7.27E-09
pr158	2.27E-15	2.28E-15	2.30E-15	ru100	3.23E-03	2.13E-02	5.25E-02	se 87	1.72E-09	1.72E-09	1.72E-09
pr159	7.84E-17	7.89E-17	7.94E-17	ru101	1.74E-01	4.21E-01	6.55E-01	se 88	2.25E-10	2.25E-10	2.25E-10
pu236	4.39E-06	7.34E-06	9.16E-06	ru102	1.86E-01	4.76E-01	7.77E-01	se 89	2.52E-11	2.53E-11	2.53E-11
pu237	6.29E-06	6.32E-06	6.35E-06	ru103	3.40E-02	3.46E-02	3.52E-02	se 90	2.99E-12	3.00E-12	3.01E-12
pu237m	6.13E-14	6.20E-14	6.25E-14	ru104	1.81E-01	4.50E-01	7.15E-01	se 91	7.97E-13	8.00E-13	8.03E-13
pu238	1.46E+00	1.41E+00	1.36E+00	ru105	1.33E-04	1.35E-04	1.37E-04	se 92	2.89E-14	2.90E-14	2.91E-14
pu239	2.95E+01	2.82E+01	2.69E+01	ru106	9.81E-02	1.65E-01	1.95E-01	se 93	6.29E-16	6.31E-16	6.34E-16
pu240	1.98E+01	1.91E+01	1.84E+01	ru107	1.14E-06	1.15E-06	1.15E-06	se 94	6.86E-17	6.88E-17	6.88E-17
pu241	2.63E+00	2.60E+00	2.55E+00	ru108	9.33E-07	9.33E-07	9.33E-07	sm143	1.76E-27	1.11E-25	7.55E-25
pu242	4.60E+00	4.41E+00	4.21E+00	ru109	7.54E-08	7.55E-08	7.56E-08	sm143m	9.00E-29	5.66E-27	3.85E-26
pu243	1.20E-04	1.20E-04	1.19E-04	ru110	1.31E-08	1.31E-08	1.31E-08	sm144	2.53E-17	1.52E-15	1.00E-14
pu244	3.64E-05	9.09E-05	1.45E-04	ru111	1.04E-09	1.04E-09	1.04E-09	sm145	1.24E-12	4.99E-11	2.26E-10
pu245	9.05E-10	2.36E-09	3.91E-09	ru112	3.52E-10	3.53E-10	3.53E-10	sm146	2.20E-07	3.64E-06	1.23E-05
pu246	3.39E-19	6.25E-18	2.28E-17	ru113	7.29E-11	7.30E-11	7.30E-11	sm147	8.47E-03	4.74E-02	1.01E-01
pu247	1.78E-21	3.44E-20	1.30E-19	ru114	1.96E-11	1.96E-11	1.96E-11	sm148	2.71E-03	2.02E-02	5.02E-02
rb 79	1.48E-27	5.19E-26	2.26E-25	ru115	6.75E-12	6.77E-12	6.79E-12	sm149	5.23E-02	1.20E-01	1.77E-01
rb 81	6.97E-17	6.99E-17	6.95E-17	ru116	3.98E-13	3.99E-13	4.00E-13	sm150	3.78E-03	2.30E-02	5.41E-02
rb 83	2.30E-10	2.46E-10	2.45E-10	ru117	4.07E-14	4.09E-14	4.10E-14	sm151	3.12E-02	6.93E-02	1.00E-01
rb 84	2.85E-09	6.95E-09	1.13E-08	ru118	6.34E-15	6.37E-15	6.39E-15	sm152	2.86E-02	7.93E-02	1.36E-01
rb 85	1.08E-02	2.70E-02	4.32E-02	ru119	7.86E-16	7.90E-16	7.92E-16	sm153	1.64E-04	1.81E-04	2.01E-04
rb 86	1.13E-05	3.04E-05	5.10E-05	ru120	6.80E-17	6.83E-17	6.86E-17	sm154	1.22E-02	3.02E-02	4.78E-02
rb 86m	6.30E-11	1.52E-10	2.48E-10	sb113	0.00E+00	0.00E+00	0.00E+00	sm155	5.90E-07	6.09E-07	6.29E-07
rb 87	2.61E-02	6.51E-02	1.04E-01	sb115	1.77E-25	6.22E-24	2.70E-23	sm156	1.04E-05	1.04E-05	1.04E-05
rb 88	1.84E-06	1.84E-06	1.84E-06	sb117	2.55E-17	2.56E-17	2.57E-17	sm157	9.40E-08	9.42E-08	9.43E-08
rb 89	2.07E-06	2.07E-06	2.06E-06	sb118	1.35E-17	1.35E-17	1.36E-17	sm158	3.47E-08	3.48E-08	3.49E-08
rb 90	3.39E-07	3.38E-07	3.38E-07	sb118m	1.90E-15	1.91E-15	1.92E-15	sm159	5.27E-10	5.29E-10	5.31E-10
rb 90m	1.55E-07	1.55E-07	1.54E-07	sb119	1.08E-12	1.08E-12	1.09E-12	sm160	1.54E-10	1.55E-10	1.55E-10
rb 91	1.79E-07	1.78E-07	1.78E-07	sb120	8.22E-13	1.97E-12	3.16E-12	sm161	1.88E-11	1.90E-11	1.91E-11
rb 92	1.34E-08	1.34E-08	1.34E-08	sb120m	2.47E-10	5.26E-10	8.14E-10	sm162	1.47E-12	1.48E-12	1.49E-12
rb 93	1.45E-08	1.45E-08	1.45E-08	sb121	1.60E-03	3.93E-03	6.16E-03	sm163	1.24E-13	1.24E-13	1.25E-13
rb 94	4.00E-09	4.00E-09	4.00E-09	sb122	6.04E-07	1.51E-06	2.45E-06	sm164	9.63E-15	9.70E-15	9.77E-15
rb 95	2.97E-10	2.97E-10	2.97E-10	sb122m	5.27E-11	1.15E-10	1.80E-10	sm165	5.59E-16	5.61E-16	5.64E-16
rb 96	5.72E-11	5.74E-11	5.75E-11	sb123	1.94E-03	5.04E-03	8.10E-03	sr 83	8.83E-17	9.53E-17	1.06E-16
rb 97	5.52E-12	5.54E-12	5.56E-12	sb124	6.80E-06	2.02E-05	3.46E-05	sr 84	4.11E-10	2.45E-09	5.97E-09
rb 98	1.76E-12	1.77E-12	1.78E-12	sb124m	1.62E-11	2.00E-11	2.40E-11	sr 85	5.57E-11	1.78E-10	4.24E-10
rb 99	1.62E-13	1.63E-13	1.63E-13	sb125	3.68E-03	7.77E-03	1.07E-02	sr 85m	2.15E-14	4.87E-14	9.97E-14
rb100	1.81E-14	1.76E-14	1.71E-14	sb126	3.70E-06	5.04E-06	6.10E-06	sr 86	6.57E-05	4.63E-04	1.18E-03
rb101	2.57E-16	2.58E-16	2.59E-16	sb126m	3.88E-09	4.18E-09	4.42E-09	sr 87	5.82E-07	3.46E-06	1.06E-05
rb102	3.43E-17	3.44E-17	3.45E-17	sb127	2.63E-04	2.62E-04	2.62E-04	sr 87m	1.88E-10	1.09E-09	2.81E-09
rh 99	2.69E-17	3.35E-17	3.28E-17	sb128	3.86E-06	3.84E-06	3.82E-06	sr 88	3.41E-02	8.51E-02	1.36E-01
rh 99m	3.54E-29	6.19E-28	2.07E-27	sb128m	7.38E-07	7.35E-07	7.33E-07	sr 89	9.91E-03	9.99E-03	9.97E-03
rh101	1.23E-12	1.63E-11	5.25E-11	sb129	3.74E-05	3.73E-05	3.72E-05	sr 90	5.48E-02	1.34E-01	2.12E-01
rh101m	2.28E-13	1.27E-12	2.80E-12	sb129m	3.01E-08	3.00E-08	2.99E-08	sr 91	1.18E-04	1.18E-04	1.17E-04
rh102	2.58E-07	1.32E-06	2.57E-06	sb130	4.18E-06	4.17E-06	4.16E-06	sr 92	3.96E-05	3.95E-05	3.94E-05
rh102m	1.62E-07	1.15E-06	2.72E-06	sb130m	8.17E-07	8.15E-07	8.13E-07	sr 93	2.21E-06	2.20E-06	2.20E-06
rh103	1.61E-01	4.39E-01	7.04E-01	sb131	7.16E-06	7.15E-06	7.14E-06	sr 94	3.74E-07	3.74E-07	3.73E-07
rh103m	3.34E-05	3.40E-05	3.46E-05	sb132	6.84E-07	6.83E-07	6.82E-07	sr 95	1.08E-07	1.08E-07	1.08E-07
rh104	1.50E-08	4.28E-08	7.13E-08	sb132m	3.77E-07	3.77E-07	3.77E-07	sr 96	3.60E-09	3.60E-09	3.59E-09
rh104m	7.34E-09	2.09E-08	3.49E-08	sb133	4.95E-07	4.95E-07	4.96E-07	sr 97	7.02E-10	7.02E-10	7.02E-10
rh105	1.06E-03	1.07E-03	1.09E-03	sb134	5.69E-10	5.71E-10	5.72E-10	sr 98	5.41E-10	5.42E-10	5.43E-10
rh105m	9.43E-08	9.57E-08	9.72E-08	sb134m	6.88E-09	6.90E-09	6.91E-09	sr 99	6.42E-11	6.45E-11	6.47E-11
rh106	9.19E-08	1.55E-07	1.82E-07	sb135	6.36E-10	6.38E-10	6.40E-10	sr100	1.27E-11	1.27E-11	1.28E-11
rh106m	6.76E-09	6.91E-09	7.06E-09	sb136	6.08E-11	6.11E-11	6.13E-11	sr101	1.06E-12	1.06E-12	1.06E-12
rh107	6.71E-06	6.73E-06	6.74E-06	sb137	4.52E-12	4.53E-12	4.53E-12	sr102	7.65E-14	7.68E-14	7.71E-14
rh108	5.79E-08	5.79E-08	5.79E-08	sb138	1.69E-13	1.70E-13	1.70E-13	sr103	2.13E-15	2.14E-15	2.14E-15
rh108m	1.03E-08	1.02E-08	1.02E-08	sb139	9.29E-15	9.33E-15	9.36E-15	sr104	1.54E-16	1.54E-16	1.55E-16
rh109	1.82E-07	1.83E-07	1.83E-07	se 72	6.53E-28	2.88E-27	6.52E-27	sr105	3.84E-17	3.86E-17	3.87E-17
rh110	1.19E-10	1.20E-10	1.21E-10	se 73	1.08E-20	4.41E-20	9.55E-20	tc 93	0.00E+00	0.00E+00	0.00E+00
rh110m	3.32E-08	3.33E-08	3.34E-08	se 73m	5.97E-22	2.45E-21	5.29E-21	tc 95	7.14E-17	8.55E-17	8.36E-17
rh111	6.52E-09	6.54E-09	6.57E-09	se 74	4.31E-11	1.69E-10	3.52E-10	tc 95m	8.50E-16	1.21E-15	1.21E-15
rh112	6.08E-10	6.09E-10	6.11E-10	se 75	8.92E-13	3.22E-12	7.37E-12	tc 96	1.31E-17	5.62E-17	1.41E-16
rh113	5.09E-10	5.10E-10	5.11E-10	se 76	4.88E-07	2.87E-06	6.92E-06	tc 97	1.52E-10	6.68E-10	1.65E-09
rh114	1.92E-10	1.92E-10	1.92E-10	se 77	1.75E-04	4.31E-04	6.78E-04	tc 97m	3.52E-11	5.77E-11	9.12E-11
rh115	5.49E-11	5.49E-11	5.49E-11	se 77m	5.29E-13	5.34E-13	5.45E-13	tc 98	9.33E-07	6.02E-06	1.47E-05
rh116	1.62E-11	1.62E-11	1.62E-11	se 78	4.23E-04	1.06E-03	1.70E-03	tc 99	1.67E-01	4.08E-01	6.38E-01
rh117	3.88E-12	3.89E-12	3.90E-12	se 79	9.67E-04	2.40E-03	3.82E-03	tc 99m	1.66E-04	1.68E-04	1.69E-04

Table A - 1: Fuel Batch Pin Radionuclide Inventory at Time = 0 (cont.)

Isotope	Batch A	Batch B	Batch C	Isotope	Batch A	Batch B	Batch C
tc100	5.11E-09	1.31E-08	2.12E-08	xe139	2.87E-07	2.87E-07	2.86E-07
tc101	7.71E-06	7.76E-06	7.82E-06	xe140	6.08E-08	6.09E-08	6.09E-08
tc102	4.89E-08	4.88E-08	4.87E-08	xe141	3.24E-09	3.25E-09	3.25E-09
tc102m	7.90E-09	7.85E-09	7.80E-09	xe142	8.51E-10	8.55E-10	8.57E-10
tc103	5.42E-07	5.41E-07	5.40E-07	xe143	4.37E-11	4.39E-11	4.41E-11
tc104	1.01E-05	1.01E-05	1.01E-05	xe144	3.83E-11	3.84E-11	3.86E-11
tc105	3.72E-06	3.72E-06	3.71E-06	xe145	6.33E-13	6.35E-13	6.38E-13
tc106	2.23E-07	2.23E-07	2.23E-07	xe146	8.69E-14	8.73E-14	8.76E-14
tc107	8.57E-08	8.58E-08	8.58E-08	xe147	5.57E-16	5.60E-16	5.63E-16
tc108	9.15E-09	9.18E-09	9.20E-09	zr 87	3.90E-20	4.71E-20	4.59E-20
tc109	6.30E-10	6.32E-10	6.34E-10	zr 88	2.67E-14	3.01E-14	3.01E-14
tc110	1.34E-10	1.35E-10	1.35E-10	zr 89	4.75E-12	3.20E-11	8.13E-11
tc111	1.00E-11	1.01E-11	1.01E-11	zr 89m	3.08E-16	2.10E-15	5.31E-15
tc112	2.62E-12	2.63E-12	2.64E-12	zr 90	6.11E-04	3.97E-03	9.73E-03
tc113	3.98E-13	4.00E-13	4.01E-13	zr 90m	1.16E-14	3.60E-14	6.21E-14
tc114	1.39E-13	1.39E-13	1.39E-13	zr 91	5.01E-02	1.50E-01	2.49E-01
tc115	1.00E-14	1.01E-14	1.01E-14	zr 92	8.08E-02	2.02E-01	3.23E-01
tc116	1.10E-15	1.10E-15	1.10E-15	zr 93	1.01E-01	2.50E-01	3.99E-01
tc117	1.80E-17	1.81E-17	1.82E-17	zr 94	1.13E-01	2.82E-01	4.53E-01
tc118	6.46E-18	6.49E-18	6.51E-18	zr 95	3.46E-02	3.56E-02	3.56E-02
tc115	0.00E+00	0.00E+00	0.00E+00	zr 96	1.35E-01	3.37E-01	5.38E-01
te117	3.79E-33	4.17E-33	4.71E-33	zr 97	4.45E-04	4.45E-04	4.45E-04
te118	1.72E-23	1.82E-23	1.97E-23	zr 98	2.41E-07	2.40E-07	2.39E-07
te119	2.70E-17	2.72E-17	2.73E-17	zr 99	1.62E-08	1.61E-08	1.61E-08
te120	1.04E-12	2.58E-12	4.10E-12	zr100	5.36E-08	5.35E-08	5.35E-08
te121	1.20E-11	6.73E-11	1.74E-10	zr101	1.04E-08	1.04E-08	1.04E-08
te121m	3.75E-11	2.40E-10	6.60E-10	zr102	7.81E-09	7.82E-09	7.83E-09
te122	2.49E-05	1.57E-04	3.83E-04	zr103	1.25E-09	1.26E-09	1.26E-09
te123	1.77E-07	2.95E-06	1.10E-05	zr104	3.61E-10	3.63E-10	3.64E-10
te123m	5.96E-08	4.99E-07	1.39E-06	zr105	3.17E-11	3.18E-11	3.19E-11
te124	1.23E-05	9.35E-05	2.44E-04	zr106	4.65E-13	4.69E-13	4.72E-13
te125	3.84E-04	2.34E-03	5.28E-03	zr107	2.11E-14	2.12E-14	2.13E-14
te125m	3.68E-05	9.35E-05	1.34E-04	zr108	5.74E-16	5.77E-16	5.79E-16
te126	1.14E-04	3.74E-04	7.49E-04	zr109	5.62E-17	5.64E-17	5.66E-17
te127	2.59E-05	2.63E-05	2.63E-05	zr110	2.17E-18	2.18E-18	2.19E-18
te127m	1.06E-03	1.19E-03	1.19E-03				
te128	2.49E-02	6.20E-02	9.91E-02				
te129	9.39E-06	9.39E-06	9.38E-06				
te129m	1.11E-03	1.11E-03	1.11E-03				
te130	8.28E-02	2.07E-01	3.30E-01				
te131	8.71E-06	8.70E-06	8.69E-06				
te131m	1.82E-04	1.81E-04	1.80E-04				
te132	2.66E-03	2.65E-03	2.64E-03				
te133	4.84E-06	4.83E-06	4.82E-06				
te133m	2.00E-05	1.99E-05	1.99E-05				
te134	2.55E-05	2.54E-05	2.54E-05				
te135	1.05E-07	1.05E-07	1.05E-07				
te136	3.74E-08	3.75E-08	3.76E-08				
te137	1.66E-09	1.67E-09	1.67E-09				
te138	2.51E-10	2.53E-10	2.54E-10				
te139	1.14E-11	1.14E-11	1.15E-11				
te140	1.45E-12	1.46E-12	1.46E-12				
te141	2.69E-13	2.70E-13	2.71E-13				
te142	4.54E-15	4.56E-15	4.58E-15				
xe124	5.82E-21	1.30E-19	5.15E-19				
xe125	8.67E-16	6.76E-15	1.78E-14				
xe125m	2.08E-19	1.62E-18	4.27E-18				
xe126	3.55E-08	2.65E-07	6.74E-07				
xe127	4.56E-10	4.08E-09	1.11E-08				
xe127m	2.22E-15	1.62E-14	4.22E-14				
xe128	2.34E-04	1.62E-03	4.07E-03				
xe129	8.79E-07	1.71E-05	6.48E-05				
xe129m	1.12E-08	8.51E-08	2.23E-07				
xe130	6.07E-04	3.65E-03	8.89E-03				
xe131	1.31E-01	3.29E-01	5.21E-01				
xe131m	7.71E-05	7.72E-05	7.75E-05				
xe132	1.94E-01	4.92E-01	7.93E-01				
xe133	5.77E-03	5.79E-03	5.82E-03				
xe133m	8.10E-05	8.26E-05	8.45E-05				
xe134	2.88E-01	7.18E-01	1.14E+00				
xe134m	8.38E-11	8.33E-11	8.29E-11				
xe135	4.75E-04	4.76E-04	4.77E-04				
xe135m	2.98E-06	2.97E-06	2.97E-06				
xe136	2.70E-01	6.74E-01	1.08E+00				
xe137	2.71E-06	2.71E-06	2.71E-06				
xe138	8.88E-06	8.87E-06	8.86E-06				

Table A - 2: Fuel Batch Pin Radionuclide Inventory – PLOF+ (Decayed)

Inventory Per Pin (g)											
Isotope	Batch A	Batch B	Batch C	Isotope	Batch A	Batch B	Batch C	Isotope	Batch A	Batch B	Batch C
AM239	3.51E-16	3.75E-16	4.89E-16	CE152	0.00E+00	0.00E+00	0.00E+00	I134	6.46E-17	6.44E-16	9.57E-14
AM240	1.39E-10	1.30E-10	1.28E-10	CE153	0.00E+00	0.00E+00	0.00E+00	I134M	0.00E+00	0.00E+00	0.00E+00
AM241	2.12E-03	1.84E-03	1.59E-03	CE154	0.00E+00	0.00E+00	0.00E+00	I135	1.06E-06	1.44E-06	2.79E-06
AM242	1.59E-07	1.62E-07	1.93E-07	CE155	0.00E+00	0.00E+00	0.00E+00	I136	0.00E+00	0.00E+00	0.00E+00
AM242M	0.00E+00	0.00E+00	0.00E+00	CE156	0.00E+00	0.00E+00	0.00E+00	I136M	0.00E+00	0.00E+00	0.00E+00
AM243	1.08E-03	1.08E-03	1.08E-03	CE157	0.00E+00	0.00E+00	0.00E+00	I137	0.00E+00	0.00E+00	0.00E+00
AM244	1.55E-09	1.98E-09	3.18E-09	CM241	1.16E-11	1.51E-11	1.49E-11	I138	0.00E+00	0.00E+00	0.00E+00
AM244M	0.00E+00	0.00E+00	0.00E+00	CM242	9.69E-05	1.12E-04	1.05E-04	I139	0.00E+00	0.00E+00	0.00E+00
AM245	2.73E-14	8.62E-14	2.16E-13	CM243	5.21E-06	6.05E-06	6.63E-06	I140	0.00E+00	0.00E+00	0.00E+00
AM246	5.43E-25	9.80E-24	3.60E-23	CM244	5.46E-04	6.08E-04	6.64E-04	I141	0.00E+00	0.00E+00	0.00E+00
BA132	3.67E-11	2.36E-10	3.83E-10	CM245	1.17E-04	1.17E-04	1.21E-04	I142	0.00E+00	0.00E+00	0.00E+00
BA133	3.73E-11	2.56E-09	1.83E-08	CM246	6.63E-05	6.69E-05	6.74E-05	I143	0.00E+00	0.00E+00	0.00E+00
BA134	6.18E-07	8.58E-06	1.86E-05	CM247	2.08E-06	4.53E-06	6.44E-06	I144	0.00E+00	0.00E+00	0.00E+00
BA135	1.27E-10	1.95E-09	7.58E-09	CM248	2.40E-08	1.42E-07	3.25E-07	I145	0.00E+00	0.00E+00	0.00E+00
BA135M	6.95E-11	1.65E-09	9.82E-09	CM249	8.78E-23	3.59E-21	5.15E-19	KR 77	0.00E+00	0.00E+00	0.00E+00
BA136	3.47E-06	1.70E-05	2.56E-05	CM250	6.17E-16	1.06E-14	3.81E-14	KR 78	2.49E-17	2.13E-16	3.98E-16
BA136M	2.13E-12	1.15E-11	2.24E-11	CM251	0.00E+00	0.00E+00	0.00E+00	KR 79	3.18E-16	1.14E-15	2.06E-15
BA137	3.16E-06	1.88E-05	2.89E-05	CO 72	0.00E+00	0.00E+00	0.00E+00	KR 79M	0.00E+00	0.00E+00	0.00E+00
BA137M	5.75E-09	3.77E-08	7.42E-08	CO 73	0.00E+00	0.00E+00	0.00E+00	KR 80	1.41E-08	1.23E-07	2.73E-07
BA138	1.21E-02	6.04E-02	1.45E-01	CO 74	0.00E+00	0.00E+00	0.00E+00	KR 81	9.81E-10	7.35E-09	1.63E-08
BA139	4.35E-13	4.10E-12	1.39E-10	CO 75	0.00E+00	0.00E+00	0.00E+00	KR 81M	0.00E+00	0.00E+00	0.00E+00
BA140	5.65E-04	1.14E-03	1.73E-03	CS132	1.20E-08	8.54E-08	1.80E-07	KR 82	1.77E-05	2.12E-04	5.28E-04
BA141	0.00E+00	0.00E+00	0.00E+00	CS133	3.78E-02	2.49E-01	4.89E-01	KR 83	2.12E-03	1.22E-02	2.06E-02
BA142	0.00E+00	0.00E+00	0.00E+00	CS134	5.05E-04	7.71E-03	2.14E-02	KR 83M	9.79E-11	2.42E-10	1.78E-09
BA143	0.00E+00	0.00E+00	0.00E+00	CS134M	2.83E-11	3.89E-10	3.60E-09	KR 84	3.72E-03	2.18E-02	3.74E-02
BA144	0.00E+00	0.00E+00	0.00E+00	CS135	4.25E-02	2.80E-01	5.56E-01	KR 85	9.12E-04	5.09E-03	8.39E-03
BA145	0.00E+00	0.00E+00	0.00E+00	CS135M	5.80E-20	1.53E-18	2.78E-16	KR 85M	2.43E-08	8.88E-08	2.54E-07
BA146	0.00E+00	0.00E+00	0.00E+00	CS136	4.76E-05	2.57E-04	5.00E-04	KR 86	6.00E-03	3.49E-02	5.98E-02
BA147	0.00E+00	0.00E+00	0.00E+00	CS137	3.76E-02	2.46E-01	4.85E-01	KR 87	5.12E-14	5.81E-13	1.96E-11
BA148	0.00E+00	0.00E+00	0.00E+00	CS138	1.09E-23	1.15E-21	4.73E-18	KR 88	2.14E-09	1.01E-08	5.07E-08
BA149	0.00E+00	0.00E+00	0.00E+00	CS138M	0.00E+00	0.00E+00	0.00E+00	KR 89	0.00E+00	0.00E+00	0.00E+00
BA150	0.00E+00	0.00E+00	0.00E+00	CS139	0.00E+00	0.00E+00	0.00E+00	KR 90	0.00E+00	0.00E+00	0.00E+00
BA151	0.00E+00	0.00E+00	0.00E+00	CS140	0.00E+00	0.00E+00	0.00E+00	KR 91	0.00E+00	0.00E+00	0.00E+00
BA152	0.00E+00	0.00E+00	0.00E+00	CS141	0.00E+00	0.00E+00	0.00E+00	KR 92	0.00E+00	0.00E+00	0.00E+00
BR 79	3.76E-13	8.48E-13	1.06E-12	CS142	0.00E+00	0.00E+00	0.00E+00	KR 93	0.00E+00	0.00E+00	0.00E+00
BR 79M	0.00E+00	0.00E+00	0.00E+00	CS143	0.00E+00	0.00E+00	0.00E+00	KR 94	0.00E+00	0.00E+00	0.00E+00
BR 80	1.49E-15	3.48E-15	1.26E-14	CS144	0.00E+00	0.00E+00	0.00E+00	KR 95	0.00E+00	0.00E+00	0.00E+00
BR 80M	2.12E-14	4.96E-14	1.79E-13	CS145	0.00E+00	0.00E+00	0.00E+00	KR 96	0.00E+00	0.00E+00	0.00E+00
BR 81	2.65E-09	2.65E-09	2.64E-09	CS146	0.00E+00	0.00E+00	0.00E+00	KR 97	0.00E+00	0.00E+00	0.00E+00
BR 82	3.30E-08	7.74E-08	1.38E-07	CS147	0.00E+00	0.00E+00	0.00E+00	KR 98	0.00E+00	0.00E+00	0.00E+00
BR 82M	0.00E+00	0.00E+00	0.00E+00	CS148	0.00E+00	0.00E+00	0.00E+00	LA138	4.93E-09	2.50E-08	5.82E-08
BR 83	3.05E-11	7.09E-11	4.43E-10	CS149	0.00E+00	0.00E+00	0.00E+00	LA139	3.88E-06	8.41E-06	1.19E-05
BR 84	8.66E-26	3.88E-24	1.53E-20	CS150	0.00E+00	0.00E+00	0.00E+00	LA140	3.33E-05	6.13E-05	7.60E-05
BR 84M	0.00E+00	0.00E+00	0.00E+00	EU149	3.21E-14	1.35E-13	1.72E-13	LA141	2.90E-09	8.88E-09	3.88E-08
BR 85	0.00E+00	0.00E+00	0.00E+00	EU150	0.00E+00	0.00E+00	0.00E+00	LA142	2.43E-13	1.67E-12	4.16E-11
BR 86	0.00E+00	0.00E+00	0.00E+00	EU151	8.76E-10	1.77E-09	1.99E-09	LA143	0.00E+00	0.00E+00	0.00E+00
BR 86M	0.00E+00	0.00E+00	0.00E+00	EU152	8.15E-07	2.82E-05	1.05E-04	LA144	0.00E+00	0.00E+00	0.00E+00
BR 87	0.00E+00	0.00E+00	0.00E+00	EU152M	2.13E-10	3.80E-09	1.62E-08	LA145	0.00E+00	0.00E+00	0.00E+00
BR 88	0.00E+00	0.00E+00	0.00E+00	EU153	6.20E-08	6.34E-08	5.76E-08	LA146	0.00E+00	0.00E+00	0.00E+00
BR 89	0.00E+00	0.00E+00	0.00E+00	EU154	1.94E-04	2.89E-03	7.92E-03	LA147	0.00E+00	0.00E+00	0.00E+00
BR 90	0.00E+00	0.00E+00	0.00E+00	EU155	1.18E-03	7.24E-03	1.39E-02	LA148	0.00E+00	0.00E+00	0.00E+00
BR 91	0.00E+00	0.00E+00	0.00E+00	EU156	6.21E-05	1.87E-04	2.63E-04	LA149	0.00E+00	0.00E+00	0.00E+00
BR 92	0.00E+00	0.00E+00	0.00E+00	EU157	3.89E-07	1.19E-06	1.98E-06	LA150	0.00E+00	0.00E+00	0.00E+00
BR 93	0.00E+00	0.00E+00	0.00E+00	EU158	1.45E-20	5.37E-19	2.08E-16	LA151	0.00E+00	0.00E+00	0.00E+00
BR 94	0.00E+00	0.00E+00	0.00E+00	EU159	0.00E+00	0.00E+00	0.00E+00	LA152	0.00E+00	0.00E+00	0.00E+00
BR 95	0.00E+00	0.00E+00	0.00E+00	EU160	0.00E+00	0.00E+00	0.00E+00	LA153	0.00E+00	0.00E+00	0.00E+00
BR 96	0.00E+00	0.00E+00	0.00E+00	EU161	0.00E+00	0.00E+00	0.00E+00	LA154	0.00E+00	0.00E+00	0.00E+00
CE139	8.25E-09	3.39E-08	6.32E-08	EU162	0.00E+00	0.00E+00	0.00E+00	LA155	0.00E+00	0.00E+00	0.00E+00
CE140	1.05E-05	1.72E-05	1.63E-05	EU163	0.00E+00	0.00E+00	0.00E+00	MO 95	4.77E-07	4.61E-07	3.61E-07
CE141	2.89E-04	2.90E-04	2.92E-04	EU164	0.00E+00	0.00E+00	0.00E+00	MO 96	1.56E-09	1.60E-09	1.41E-09
CE142	1.96E-03	4.90E-03	7.82E-03	EU165	0.00E+00	0.00E+00	0.00E+00	MO 97	3.48E-07	3.32E-07	2.89E-07
CE143	5.61E-06	5.97E-06	6.83E-06	I127	5.96E-07	5.54E-07	4.37E-07	MO 98	4.34E-10	5.41E-10	6.75E-10
CE144	1.10E-03	1.70E-03	1.91E-03	I128	0.00E+00	1.19E-29	7.33E-25	MO 99	1.49E-06	1.55E-06	1.67E-06
CE145	0.00E+00	0.00E+00	0.00E+00	I129	4.55E-03	1.13E-02	1.79E-02	MO100	7.06E-11	7.30E-11	7.61E-11
CE146	0.00E+00	0.00E+00	0.00E+00	I130	3.87E-08	1.11E-07	2.56E-07	MO101	0.00E+00	0.00E+00	0.00E+00
CE147	0.00E+00	0.00E+00	0.00E+00	I130M	0.00E+00	0.00E+00	0.00E+00	MO102	0.00E+00	0.00E+00	0.00E+00
CE148	0.00E+00	0.00E+00	0.00E+00	I131	4.27E-04	4.31E-04	4.40E-04	MO103	0.00E+00	0.00E+00	0.00E+00
CE149	0.00E+00	0.00E+00	0.00E+00	I132	6.07E-07	6.23E-07	6.64E-07	MO104	0.00E+00	0.00E+00	0.00E+00
CE150	0.00E+00	0.00E+00	0.00E+00	I133	3.41E-05	3.74E-05	4.61E-05	MO105	0.00E+00	0.00E+00	0.00E+00
CE151	0.00E+00	0.00E+00	0.00E+00	I133M	0.00E+00	0.00E+00	0.00E+00	MO106	0.00E+00	0.00E+00	0.00E+00

Table A - 2: Fuel Batch Pin Radionuclide Inventory – PLOF+ (Decayed) (cont.)

Inventory Per Pin (g)											
Isotope	Batch A	Batch B	Batch C	Isotope	Batch A	Batch B	Batch C	Isotope	Batch A	Batch B	Batch C
MO107	0.00E+00	0.00E+00	0.00E+00	PD105	5.45E-07	5.15E-07	4.29E-07	PU237	6.16E-09	6.21E-09	6.26E-09
MO108	0.00E+00	0.00E+00	0.00E+00	PD106	2.45E-07	3.75E-07	3.46E-07	PU238	1.47E-03	1.42E-03	1.36E-03
MO109	0.00E+00	0.00E+00	0.00E+00	PD107	9.81E-05	2.35E-04	3.62E-04	PU239	2.96E-02	2.82E-02	2.69E-02
MO110	0.00E+00	0.00E+00	0.00E+00	PD107M	0.00E+00	0.00E+00	0.00E+00	PU240	1.98E-02	1.91E-02	1.84E-02
MO111	0.00E+00	0.00E+00	0.00E+00	PD108	1.01E-09	1.01E-09	1.01E-09	PU241	2.63E-03	2.60E-03	2.55E-03
MO112	0.00E+00	0.00E+00	0.00E+00	PD109	2.23E-08	2.70E-08	3.91E-08	PU242	4.61E-03	4.41E-03	4.21E-03
MO113	0.00E+00	0.00E+00	0.00E+00	PD109M	0.00E+00	0.00E+00	0.00E+00	PU243	1.39E-09	2.08E-09	5.03E-09
MO114	0.00E+00	0.00E+00	0.00E+00	PD110	4.66E-11	4.67E-11	4.68E-11	PU244	3.64E-08	9.09E-08	1.45E-07
MO115	0.00E+00	0.00E+00	0.00E+00	PD111	7.66E-14	1.66E-13	4.98E-13	PU245	1.13E-13	3.55E-13	8.89E-13
NB 91	1.41E-15	3.72E-15	6.02E-15	PD111M	1.58E-12	3.42E-12	1.03E-11	PU246	3.39E-22	6.11E-21	2.24E-20
NB 92	1.10E-13	2.82E-13	4.59E-13	PD112	7.56E-09	8.40E-09	1.05E-08	RB 85	2.86E-06	7.22E-06	7.86E-06
NB 93	1.23E-14	4.03E-14	6.33E-14	PD113	0.00E+00	0.00E+00	0.00E+00	RB 86	1.62E-06	1.17E-05	2.46E-05
NB 93M	2.14E-11	1.28E-10	3.03E-10	PD114	0.00E+00	0.00E+00	0.00E+00	RB 86M	0.00E+00	0.00E+00	0.00E+00
NB 94	5.72E-10	1.75E-09	2.94E-09	PD115	0.00E+00	0.00E+00	0.00E+00	RB 87	3.92E-03	2.61E-02	5.20E-02
NB 94M	0.00E+00	0.00E+00	0.00E+00	PD116	0.00E+00	0.00E+00	0.00E+00	RB 88	2.50E-10	1.18E-09	5.92E-09
NB 95	1.82E-05	1.94E-05	1.94E-05	PD117	0.00E+00	0.00E+00	0.00E+00	RB 89	0.00E+00	0.00E+00	0.00E+00
NB 95M	1.94E-08	2.01E-08	2.04E-08	PD118	0.00E+00	0.00E+00	0.00E+00	RB 90	0.00E+00	0.00E+00	0.00E+00
NB 96	9.88E-10	1.18E-09	1.47E-09	PD119	0.00E+00	0.00E+00	0.00E+00	RB 90M	0.00E+00	0.00E+00	0.00E+00
NB 97	8.60E-09	9.69E-09	1.26E-08	PD120	0.00E+00	0.00E+00	0.00E+00	RB 91	0.00E+00	0.00E+00	0.00E+00
NB 97M	1.12E-10	1.27E-10	1.65E-10	PD121	0.00E+00	0.00E+00	0.00E+00	RB 92	0.00E+00	0.00E+00	0.00E+00
NB 98	0.00E+00	0.00E+00	0.00E+00	PD122	0.00E+00	0.00E+00	0.00E+00	RB 93	0.00E+00	0.00E+00	0.00E+00
NB 98M	9.32E-22	9.71E-21	1.60E-18	PD123	0.00E+00	0.00E+00	0.00E+00	RB 94	0.00E+00	0.00E+00	0.00E+00
NB 99	0.00E+00	0.00E+00	0.00E+00	PD124	0.00E+00	0.00E+00	0.00E+00	RB 95	0.00E+00	0.00E+00	0.00E+00
NB 99M	0.00E+00	0.00E+00	0.00E+00	PD125	0.00E+00	0.00E+00	0.00E+00	RB 96	0.00E+00	0.00E+00	0.00E+00
NB100	0.00E+00	0.00E+00	0.00E+00	PD126	0.00E+00	0.00E+00	0.00E+00	RB 97	0.00E+00	0.00E+00	0.00E+00
NB100M	0.00E+00	0.00E+00	0.00E+00	PM145	2.05E-13	2.80E-12	8.97E-12	RB 98	0.00E+00	0.00E+00	0.00E+00
NB101	0.00E+00	0.00E+00	0.00E+00	PM146	2.46E-09	1.33E-08	2.75E-08	RB 99	0.00E+00	0.00E+00	0.00E+00
NB102	0.00E+00	0.00E+00	0.00E+00	PM147	7.33E-05	1.50E-04	2.01E-04	RB100	0.00E+00	0.00E+00	0.00E+00
NB103	0.00E+00	0.00E+00	0.00E+00	PM148	6.49E-08	1.44E-07	2.09E-07	RB101	0.00E+00	0.00E+00	0.00E+00
NB104	0.00E+00	0.00E+00	0.00E+00	PM148M	0.00E+00	0.00E+00	0.00E+00	RH102	2.58E-10	1.31E-09	2.57E-09
NB105	0.00E+00	0.00E+00	0.00E+00	PM149	3.76E-07	3.99E-07	4.43E-07	RH103	7.91E-07	7.34E-07	5.85E-07
NB106	0.00E+00	0.00E+00	0.00E+00	PM150	1.67E-14	3.68E-14	1.97E-13	RH103M	2.97E-08	3.03E-08	3.10E-08
NB107	0.00E+00	0.00E+00	0.00E+00	PM151	8.26E-08	9.04E-08	1.08E-07	RH104	0.00E+00	0.00E+00	0.00E+00
NB108	0.00E+00	0.00E+00	0.00E+00	PM152	0.00E+00	0.00E+00	0.00E+00	RH104M	0.00E+00	0.00E+00	0.00E+00
NB109	0.00E+00	0.00E+00	0.00E+00	PM152M	0.00E+00	0.00E+00	0.00E+00	RH105	6.49E-07	6.97E-07	7.99E-07
NB110	0.00E+00	0.00E+00	0.00E+00	PM153	0.00E+00	0.00E+00	0.00E+00	RH105M	7.45E-13	1.19E-12	3.25E-12
NB111	0.00E+00	0.00E+00	0.00E+00	PM154	0.00E+00	0.00E+00	0.00E+00	RH106	9.20E-11	1.55E-10	1.83E-10
NB112	0.00E+00	0.00E+00	0.00E+00	PM154M	0.00E+00	0.00E+00	0.00E+00	RH106M	2.93E-16	7.49E-16	5.62E-15
ND141	2.83E-19	5.25E-18	8.18E-17	PM155	0.00E+00	0.00E+00	0.00E+00	RH107	0.00E+00	0.00E+00	1.16E-27
ND142	3.15E-09	8.52E-09	1.24E-08	PM156	0.00E+00	0.00E+00	0.00E+00	RH108	0.00E+00	0.00E+00	0.00E+00
ND143	8.81E-07	7.91E-07	5.98E-07	PM157	0.00E+00	0.00E+00	0.00E+00	RH108M	0.00E+00	0.00E+00	0.00E+00
ND144	5.48E-05	2.42E-04	4.72E-04	PM158	0.00E+00	0.00E+00	0.00E+00	RH109	0.00E+00	0.00E+00	0.00E+00
ND145	1.51E-07	1.50E-07	1.44E-07	PM159	0.00E+00	0.00E+00	0.00E+00	RH109M	0.00E+00	0.00E+00	0.00E+00
ND146	5.28E-08	5.28E-08	5.29E-08	PM160	0.00E+00	0.00E+00	0.00E+00	RH110	0.00E+00	0.00E+00	0.00E+00
ND147	3.97E-06	4.04E-06	4.17E-06	PM161	0.00E+00	0.00E+00	0.00E+00	RH110M	0.00E+00	0.00E+00	0.00E+00
ND148	2.06E-09	2.06E-09	2.07E-09	PM162	0.00E+00	0.00E+00	0.00E+00	RH111	0.00E+00	0.00E+00	0.00E+00
ND149	5.20E-14	1.70E-13	2.19E-12	PR139	5.33E-21	9.94E-21	2.65E-20	RH112	0.00E+00	0.00E+00	0.00E+00
ND150	5.05E-11	5.06E-11	5.07E-11	PR140	0.00E+00	0.00E+00	0.00E+00	RH113	0.00E+00	0.00E+00	0.00E+00
ND151	0.00E+00	0.00E+00	0.00E+00	PR141	8.29E-06	7.56E-06	5.92E-06	RH114	0.00E+00	0.00E+00	0.00E+00
ND152	0.00E+00	0.00E+00	0.00E+00	PR142	1.45E-09	4.59E-09	9.74E-09	RH115	0.00E+00	0.00E+00	0.00E+00
ND153	0.00E+00	0.00E+00	0.00E+00	PR142M	0.00E+00	0.00E+00	0.00E+00	RH116	0.00E+00	0.00E+00	0.00E+00
ND154	0.00E+00	0.00E+00	0.00E+00	PR143	1.49E-05	1.47E-05	1.40E-05	RH117	0.00E+00	0.00E+00	0.00E+00
ND155	0.00E+00	0.00E+00	0.00E+00	PR144	4.63E-08	7.17E-08	8.04E-08	RH118	0.00E+00	0.00E+00	0.00E+00
ND156	0.00E+00	0.00E+00	0.00E+00	PR144M	2.31E-10	3.58E-10	4.02E-10	RH119	0.00E+00	0.00E+00	0.00E+00
ND157	0.00E+00	0.00E+00	0.00E+00	PR145	3.83E-09	5.39E-09	1.13E-08	RH120	0.00E+00	0.00E+00	0.00E+00
ND158	0.00E+00	0.00E+00	0.00E+00	PR146	0.00E+00	2.73E-29	1.45E-24	RH121	0.00E+00	0.00E+00	0.00E+00
ND159	0.00E+00	0.00E+00	0.00E+00	PR147	0.00E+00	0.00E+00	0.00E+00	RH122	0.00E+00	0.00E+00	0.00E+00
ND160	0.00E+00	0.00E+00	0.00E+00	PR148	0.00E+00	0.00E+00	0.00E+00	RH123	0.00E+00	0.00E+00	0.00E+00
ND161	0.00E+00	0.00E+00	0.00E+00	PR149	0.00E+00	0.00E+00	0.00E+00	RU 99	1.98E-12	4.40E-12	5.37E-12
NP235	4.84E-12	8.25E-12	9.88E-12	PR150	0.00E+00	0.00E+00	0.00E+00	RU100	5.11E-12	1.31E-11	2.12E-11
NP236	2.03E-09	4.25E-09	5.84E-09	PR151	0.00E+00	0.00E+00	0.00E+00	RU101	1.57E-08	1.58E-08	1.59E-08
NP236M	1.30E-11	1.45E-11	1.79E-11	PR152	0.00E+00	0.00E+00	0.00E+00	RU102	6.34E-09	6.33E-09	6.32E-09
NP237	3.33E-04	3.26E-04	3.18E-04	PR153	0.00E+00	0.00E+00	0.00E+00	RU103	3.32E-05	3.39E-05	3.46E-05
NP238	2.21E-07	2.34E-07	2.59E-07	PR154	0.00E+00	0.00E+00	0.00E+00	RU104	1.06E-08	1.06E-08	1.06E-08
NP239	2.97E-05	3.09E-05	3.35E-05	PR155	0.00E+00	0.00E+00	0.00E+00	RU105	9.42E-10	1.51E-09	4.11E-09
NP240	5.60E-19	3.76E-18	2.26E-16	PR156	0.00E+00	0.00E+00	0.00E+00	RU106	9.78E-05	1.65E-04	1.95E-04
NP240M	6.12E-21	1.53E-20	2.45E-20	PR157	0.00E+00	0.00E+00	0.00E+00	RU107	0.00E+00	0.00E+00	0.00E+00
NP241	0.00E+00	0.00E+00	0.00E+00	PR158	0.00E+00	0.00E+00	0.00E+00	RU108	0.00E+00	0.00E+00	0.00E+00
PD102	0.00E+00	0.00E+00	0.00E+00	PR159	0.00E+00	0.00E+00	0.00E+00	RU109	0.00E+00	0.00E+00	0.00E+00
PD104	2.22E-11	6.34E-11	1.06E-10	PU236	4.39E-09	7.35E-09	9.16E-09	RU110	0.00E+00	0.00E+00	0.00E+00

Table A - 2: Fuel Batch Pin Radionuclide Inventory – PLOF+ (Decayed) (cont.)

Inventory Per Pin (g)											
Isotope	Batch A	Batch B	Batch C	Isotope	Batch A	Batch B	Batch C	Isotope	Batch A	Batch B	Batch C
RU111	0.00E+00	0.00E+00	0.00E+00	SM156	9.93E-10	1.23E-09	1.96E-09	TE133M	8.02E-18	7.11E-17	8.21E-15
RU112	0.00E+00	0.00E+00	0.00E+00	SM157	0.00E+00	0.00E+00	0.00E+00	TE134	4.23E-21	7.65E-20	4.15E-17
RU113	0.00E+00	0.00E+00	0.00E+00	SM158	2.79E-24	4.39E-23	1.75E-20	TE135	0.00E+00	0.00E+00	0.00E+00
RU114	0.00E+00	0.00E+00	0.00E+00	SM159	0.00E+00	0.00E+00	0.00E+00	TE136	0.00E+00	0.00E+00	0.00E+00
RU115	0.00E+00	0.00E+00	0.00E+00	SM160	0.00E+00	0.00E+00	0.00E+00	TE137	0.00E+00	0.00E+00	0.00E+00
RU116	0.00E+00	0.00E+00	0.00E+00	SM161	0.00E+00	0.00E+00	0.00E+00	TE138	0.00E+00	0.00E+00	0.00E+00
RU117	0.00E+00	0.00E+00	0.00E+00	SM162	0.00E+00	0.00E+00	0.00E+00	TE139	0.00E+00	0.00E+00	0.00E+00
RU118	0.00E+00	0.00E+00	0.00E+00	SM163	0.00E+00	0.00E+00	0.00E+00	TE140	0.00E+00	0.00E+00	0.00E+00
RU119	0.00E+00	0.00E+00	0.00E+00	SM164	0.00E+00	0.00E+00	0.00E+00	TE141	0.00E+00	0.00E+00	0.00E+00
RU120	0.00E+00	0.00E+00	0.00E+00	SM165	0.00E+00	0.00E+00	0.00E+00	TE142	0.00E+00	0.00E+00	0.00E+00
SB121	2.89E-16	2.73E-16	2.30E-16	SR 86	8.17E-08	5.34E-07	8.78E-07	U230	6.12E-18	3.22E-17	7.12E-17
SB122	4.30E-09	1.11E-08	1.93E-08	SR 87	9.37E-12	2.73E-10	1.39E-09	U231	6.89E-16	2.64E-15	5.08E-15
SB122M	0.00E+00	0.00E+00	0.00E+00	SR 87M	3.56E-15	2.13E-13	5.21E-12	U232	6.04E-10	2.13E-09	3.77E-09
SB123	2.20E-17	2.21E-17	2.22E-17	SR 88	5.42E-06	1.27E-05	1.37E-05	U233	9.37E-09	1.93E-08	2.60E-08
SB124	6.70E-08	1.99E-07	3.42E-07	SR 89	4.87E-04	2.46E-03	4.92E-03	U234	4.62E-04	4.34E-04	4.07E-04
SB124M	0.00E+00	0.00E+00	0.00E+00	SR 90	2.74E-03	3.36E-02	1.06E-01	U235	1.57E-04	1.39E-04	1.23E-04
SB125	3.68E-05	7.76E-05	1.07E-04	SR 91	5.79E-07	3.56E-06	1.13E-05	U236	2.41E-04	2.38E-04	2.34E-04
SB126	3.44E-08	4.72E-08	5.79E-08	SR 92	5.69E-10	5.97E-09	6.01E-08	U237	1.04E-06	1.06E-06	1.10E-06
SB126M	0.00E+00	0.00E+00	1.30E-32	SR 93	0.00E+00	0.00E+00	0.00E+00	U238	2.15E-01	2.07E-01	2.00E-01
SB127	2.07E-06	2.11E-06	2.21E-06	SR 94	0.00E+00	0.00E+00	0.00E+00	U239	0.00E+00	0.00E+00	1.26E-24
SB128	3.32E-09	4.13E-09	6.69E-09	SR 95	0.00E+00	0.00E+00	0.00E+00	U240	6.99E-19	1.75E-18	2.79E-18
SB128M	0.00E+00	0.00E+00	0.00E+00	SR 96	0.00E+00	0.00E+00	0.00E+00	U241	0.00E+00	0.00E+00	0.00E+00
SB129	2.24E-09	3.57E-09	9.82E-09	SR 97	0.00E+00	0.00E+00	0.00E+00	XE124	1.75E-21	9.10E-20	3.86E-19
SB130	1.67E-22	3.43E-21	2.47E-18	SR 98	0.00E+00	0.00E+00	0.00E+00	XE125	0.00E+00	0.00E+00	0.00E+00
SB130M	0.00E+00	0.00E+00	0.00E+00	SR 99	0.00E+00	0.00E+00	0.00E+00	XE125M	0.00E+00	0.00E+00	0.00E+00
SB131	0.00E+00	0.00E+00	1.17E-25	SR100	0.00E+00	0.00E+00	0.00E+00	XE126	1.07E-08	1.85E-07	5.05E-07
SB132	0.00E+00	0.00E+00	0.00E+00	SR101	0.00E+00	0.00E+00	0.00E+00	XE127	1.33E-10	2.79E-09	8.17E-09
SB132M	0.00E+00	0.00E+00	0.00E+00	SR102	0.00E+00	0.00E+00	0.00E+00	XE127M	0.00E+00	0.00E+00	0.00E+00
SB133	0.00E+00	0.00E+00	0.00E+00	SR103	0.00E+00	0.00E+00	0.00E+00	XE128	7.04E-05	1.14E-03	3.06E-03
SB134	0.00E+00	0.00E+00	0.00E+00	SR104	0.00E+00	0.00E+00	0.00E+00	XE129	2.64E-07	1.19E-05	4.86E-05
SB134M	0.00E+00	0.00E+00	0.00E+00	TC 98	9.33E-10	6.02E-09	1.47E-08	XE129M	2.99E-09	5.37E-08	1.54E-07
SB135	0.00E+00	0.00E+00	0.00E+00	TC 99	1.67E-04	4.09E-04	6.39E-04	XE130	1.82E-04	2.56E-03	6.67E-03
SB136	0.00E+00	0.00E+00	0.00E+00	TC 99M	1.30E-07	1.35E-07	1.45E-07	XE131	3.93E-02	2.30E-01	3.90E-01
SB137	0.00E+00	0.00E+00	0.00E+00	TC100	0.00E+00	0.00E+00	0.00E+00	XE131M	2.20E-05	5.09E-05	5.54E-05
SB138	0.00E+00	0.00E+00	0.00E+00	TC101	0.00E+00	0.00E+00	0.00E+00	XE132	5.82E-02	3.44E-01	5.95E-01
SB139	0.00E+00	0.00E+00	0.00E+00	TC102	0.00E+00	0.00E+00	0.00E+00	XE133	1.52E-03	3.53E-03	3.92E-03
SE 76	0.00E+00	0.00E+00	0.00E+00	TC102M	0.00E+00	0.00E+00	0.00E+00	XE133M	1.74E-05	4.09E-05	4.83E-05
SE 77	5.29E-15	5.34E-15	5.45E-15	TC103	0.00E+00	0.00E+00	0.00E+00	XE134	8.64E-02	5.02E-01	8.59E-01
SE 77M	0.00E+00	0.00E+00	0.00E+00	TC104	0.00E+00	0.00E+00	0.00E+00	XE134M	0.00E+00	0.00E+00	0.00E+00
SE 78	0.00E+00	0.00E+00	0.00E+00	TC105	0.00E+00	0.00E+00	0.00E+00	XE135	1.84E-05	4.36E-05	7.33E-05
SE 79	9.67E-06	2.40E-05	3.82E-05	TC106	0.00E+00	0.00E+00	0.00E+00	XE135M	6.55E-09	8.87E-09	1.72E-08
SE 79M	0.00E+00	0.00E+00	0.00E+00	TC107	0.00E+00	0.00E+00	0.00E+00	XE136	8.09E-02	4.72E-01	8.07E-01
SE 80	2.89E-13	4.34E-13	5.75E-13	TC108	0.00E+00	0.00E+00	0.00E+00	XE137	0.00E+00	0.00E+00	0.00E+00
SE 81	3.07E-20	2.53E-19	2.50E-17	TC109	0.00E+00	0.00E+00	0.00E+00	XE138	0.00E+00	0.00E+00	0.00E+00
SE 81M	6.44E-20	5.31E-19	5.24E-17	TC110	0.00E+00	0.00E+00	0.00E+00	XE139	0.00E+00	0.00E+00	0.00E+00
SE 82	0.00E+00	0.00E+00	0.00E+00	TC111	0.00E+00	0.00E+00	0.00E+00	XE140	0.00E+00	0.00E+00	0.00E+00
SE 83	0.00E+00	0.00E+00	2.76E-27	TC112	0.00E+00	0.00E+00	0.00E+00	XE141	0.00E+00	0.00E+00	0.00E+00
SE 83M	0.00E+00	0.00E+00	0.00E+00	TC113	0.00E+00	0.00E+00	0.00E+00	XE142	0.00E+00	0.00E+00	0.00E+00
SE 84	0.00E+00	0.00E+00	0.00E+00	TC114	0.00E+00	0.00E+00	0.00E+00	XE143	0.00E+00	0.00E+00	0.00E+00
SE 85	0.00E+00	0.00E+00	0.00E+00	TC115	0.00E+00	0.00E+00	0.00E+00	XE144	0.00E+00	0.00E+00	0.00E+00
SE 85M	0.00E+00	0.00E+00	0.00E+00	TC116	0.00E+00	0.00E+00	0.00E+00	XE145	0.00E+00	0.00E+00	0.00E+00
SE 86	0.00E+00	0.00E+00	0.00E+00	TC117	0.00E+00	0.00E+00	0.00E+00	XE146	0.00E+00	0.00E+00	0.00E+00
SE 87	0.00E+00	0.00E+00	0.00E+00	TC118	0.00E+00	0.00E+00	0.00E+00	XE147	0.00E+00	0.00E+00	0.00E+00
SE 88	0.00E+00	0.00E+00	0.00E+00	TE122	1.71E-09	3.94E-09	5.15E-09	Y 90	2.11E-07	2.30E-06	5.81E-06
SE 89	0.00E+00	0.00E+00	0.00E+00	TE123	1.78E-09	2.96E-08	1.10E-07	Y 90M	1.19E-15	3.98E-15	2.39E-14
SE 90	0.00E+00	0.00E+00	0.00E+00	TE123M	5.92E-10	4.95E-09	1.39E-08	Y 91	2.18E-05	4.24E-05	6.35E-05
SE 91	0.00E+00	0.00E+00	0.00E+00	TE124	1.03E-09	2.79E-09	3.74E-09	Y 91M	3.21E-08	1.97E-07	6.24E-07
SE 92	0.00E+00	0.00E+00	0.00E+00	TE125	3.16E-08	6.30E-08	6.84E-08	Y 92	1.41E-08	1.19E-07	7.41E-07
SE 93	0.00E+00	0.00E+00	0.00E+00	TE125M	3.70E-07	9.37E-07	1.35E-06	Y 93	3.38E-08	1.03E-07	2.76E-07
SM145	1.23E-15	4.98E-14	2.25E-13	TE126	2.68E-09	3.33E-09	3.18E-09	Y 94	0.00E+00	0.00E+00	7.93E-29
SM146	2.20E-10	3.64E-09	1.23E-08	TE127	2.35E-07	2.42E-07	2.50E-07	Y 95	0.00E+00	0.00E+00	0.00E+00
SM147	8.54E-06	4.76E-05	1.01E-04	TE127M	1.05E-05	1.19E-05	1.19E-05	Y 96	0.00E+00	0.00E+00	0.00E+00
SM148	2.72E-06	2.02E-05	5.02E-05	TE128	4.29E-08	4.22E-08	3.99E-08	Y 97	0.00E+00	0.00E+00	0.00E+00
SM149	5.25E-05	1.20E-04	1.77E-04	TE129	1.09E-08	1.13E-08	1.34E-08	Y 98	0.00E+00	0.00E+00	0.00E+00
SM150	6.36E-11	6.62E-11	6.86E-11	TE129M	1.09E-05	1.09E-05	1.09E-05	Y 99	0.00E+00	0.00E+00	0.00E+00
SM151	3.13E-05	6.94E-05	1.00E-04	TE130	5.00E-08	4.99E-08	4.98E-08	Y100	0.00E+00	0.00E+00	0.00E+00
SM152	1.89E-09	1.27E-08	3.10E-08	TE131	2.72E-09	2.90E-09	3.35E-09	Y101	0.00E+00	0.00E+00	0.00E+00
SM153	1.02E-07	1.18E-07	1.44E-07	TE131M	8.71E-07	9.28E-07	1.07E-06	Y102	0.00E+00	0.00E+00	0.00E+00
SM154	6.47E-11	6.48E-11	6.49E-11	TE132	2.00E-05	2.05E-05	2.16E-05	Y103	0.00E+00	0.00E+00	0.00E+00
SM155	0.00E+00	0.00E+00	2.42E-28	TE133	3.02E-19	2.68E-18	3.09E-16	Y104	0.00E+00	0.00E+00	0.00E+00

Table A - 2: Fuel Batch Pin Radionuclide Inventory – PLOF+ (Decayed) (cont.)

Inventory Per Pin (g)			
Isotope	Batch A	Batch B	Batch C
Y105	0.00E+00	0.00E+00	0.00E+00
Y106	0.00E+00	0.00E+00	0.00E+00
Y107	0.00E+00	0.00E+00	0.00E+00
ZR 90	4.09E-08	3.85E-07	7.49E-07
ZR 90M	0.00E+00	0.00E+00	0.00E+00
ZR 91	3.19E-07	4.87E-07	5.20E-07
ZR 92	7.26E-06	3.47E-05	1.90E-05
ZR 93	1.01E-04	2.51E-04	4.00E-04
ZR 94	2.56E-08	1.01E-07	1.95E-07
ZR 95	3.41E-05	3.52E-05	3.53E-05
ZR 96	2.08E-10	9.43E-10	1.85E-09
ZR 97	1.20E-07	1.36E-07	1.76E-07
ZR 98	0.00E+00	0.00E+00	0.00E+00
ZR 99	0.00E+00	0.00E+00	0.00E+00
ZR100	0.00E+00	0.00E+00	0.00E+00
ZR101	0.00E+00	0.00E+00	0.00E+00
ZR102	0.00E+00	0.00E+00	0.00E+00
ZR103	0.00E+00	0.00E+00	0.00E+00
ZR104	0.00E+00	0.00E+00	0.00E+00
ZR105	0.00E+00	0.00E+00	0.00E+00
ZR106	0.00E+00	0.00E+00	0.00E+00
ZR107	0.00E+00	0.00E+00	0.00E+00
ZR108	0.00E+00	0.00E+00	0.00E+00
ZR109	0.00E+00	0.00E+00	0.00E+00

A.2 In-Pin Radionuclide Form

Figure A - 1 through Figure A - 10 present the detailed results of the HSC in-pin radionuclide form calculations. Each figures describes the percentage of the pin inventory that is contained within the fuel matrix, in the bond sodium (in the liquid or solid state), or in the plenum as a gas. Table A - 3 contains the results of the HSC calculations for the pre- and peri-failure fuel pin conditions. The table includes the speciation and state of the radionuclides (and bond sodium) in the plenum region of the fuel pins.

PLOF+: Pre-Failure - Batch A **Figure A - 1: PLOF+: Pre-Failure – Batch A**

PLOF+: Pre-Failure - Batch B

Figure A - 2: PLOF+: Pre-Failure – Batch B

PLOF+: Pre-Failure - Batch C **Figure A - 3: PLOF+: Pre-Failure – Batch C**

PLOF+: Peri-Failure - Batch A **Figure A - 4: PLOF+: Peri-Failure – Batch A**

PLOF+: Peri-Failure - Batch B **Figure A - 5: PLOF+: Peri-Failure – Batch B**

PLOF+: Peri-Failure - Batch C **Figure A - 6: PLOF+: Peri-Failure – Batch C**

UTOP+: Pre-Failure - Batch B **Figure A - 7: UTOP+: Pre-Failure – Batch B**

UTOP+: Pre-Failure - Batch C **Figure A - 8: UTOP+: Pre-Failure – Batch C**

UTOP+: Peri-Failure - Batch B **Figure A - 9: UTOP+: Peri-Failure – Batch B**

Figure A - 10: UTOP+: Peri-Failure – Batch C

Table A - 3: HSC Fuel Pin Plenum Condition Calculation Results¹

	UTOP+			
Fuel Batch	B		C	
Timing	Pre-failure	Peri-failure	Pre-failure	Peri-failure
T (°C)	1300	1300	1229	1229
P (Mpa)	10	0.27	19	0.27
Equilibrium Species	moles	moles	moles	moles
Kr(g)	8.80E-04	1.20E-03	1.50E-03	2.00E-03
Xe(g)	1.30E-02	1.80E-02	2.00E-02	2.80E-02
Xe2(g)	1.10E-04	3.20E-07	4.00E-04	8.10E-07
Am(g)	9.70E-12	6.60E-06	2.60E-12	2.40E-06
Am Gas	9.70E-12	6.60E-06	2.60E-12	2.40E-06
Am	6.40E-06	4.40E-04	5.90E-06	3.50E-04
Am(l)	6.40E-06	4.40E-04	5.90E-06	3.50E-04
Am Condensed	6.40E-06	4.40E-04	5.90E-06	3.50E-04
Am Gas Fraction	1.50E-06	1.50E-02	4.40E-07	6.90E-03
Ba(g)	1.60E-08	2.40E-04	1.70E-08	2.90E-04
Ba2(g)	1.50E-15	4.70E-10	2.30E-15	7.00E-10
BaBr(g)	4.40E-12	1.10E-06	5.00E-12	1.40E-06
BaBr2(g)	3.50E-16	1.50E-09	4.90E-16	2.30E-09
BaI(g)	9.40E-11	4.90E-06	1.60E-10	6.30E-06
BaI2(g)	1.40E-13	2.60E-08	4.10E-13	3.90E-08
Ba Gas	1.60E-08	2.40E-04	1.70E-08	2.90E-04
Ba	0.00E+00	0.00E+00	0.00E+00	0.00E+00
BaBr2	4.80E-11	2.00E-08	1.90E-10	5.80E-08
BaI2(l)	6.70E-08	1.30E-06	4.90E-07	2.90E-06
Ba(l)	4.80E-04	7.10E-04	1.20E-03	1.30E-03
BaTe	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ba Condensed	4.80E-04	7.10E-04	1.20E-03	1.30E-03
Ba Gas Fraction	3.40E-05	2.60E-01	1.40E-05	1.90E-01
Br(g)	2.30E-17	2.80E-13	4.70E-18	7.40E-14
Br2(g)	1.80E-29	3.60E-24	1.90E-30	5.00E-25
BaBr(g)	4.40E-12	1.10E-06	5.00E-12	1.40E-06
BaBr2(g)	3.50E-16	1.50E-09	4.90E-16	2.30E-09
CeBr3(g)	1.60E-26	7.20E-15	9.50E-27	5.10E-15
EuBr2(g)	6.90E-19	8.90E-13	6.30E-19	1.00E-12
IBr(g)	6.10E-26	2.60E-21	1.10E-26	4.30E-22
LaBr3(g)	5.70E-28	2.70E-19	3.50E-28	2.60E-19
MoBr(g)	3.80E-30	6.30E-24	3.50E-31	9.10E-25
MoBr2(g)	6.00E-36	1.70E-28	5.90E-37	2.60E-29
MoBr3(g)	1.30E-45	6.30E-37	9.60E-47	7.00E-38

	PLOF+					
Fuel Batch	A		B		C	
Timing	Pre-failure	Peri-failure	Pre-failure	Peri-failure	Pre-failure	Peri-failure
T (°C)	754	754	741	741	719	719
P (MPa)	0.64	0.23	3.85	0.22	8.69	0.21
Equilibrium Species	moles	moles	moles	moles	moles	moles
Kr(g)	1.50E-04	1.50E-04	8.70E-04	8.70E-04	1.50E-03	1.50E-03
Xe(g)	3.60E-03	3.60E-03	1.30E-02	1.30E-02	2.00E-02	2.20E-02
Xe2(g)	6.60E-06	2.20E-06	1.50E-04	7.80E-06	6.50E-04	1.60E-05
Am(g)	1.10E-15	3.40E-15	3.30E-16	6.60E-15	7.90E-18	3.60E-16
Am Gas	1.10E-15	3.40E-15	3.30E-16	6.60E-15	7.90E-18	3.60E-16
Am(l)	4.60E-06	4.60E-06	4.10E-06	4.10E-06	3.30E-06	3.30E-06
Am	8.60E-06	8.60E-06	7.90E-06	7.90E-06	7.80E-06	7.80E-06
Am Condensed	1.30E-05	1.30E-05	1.20E-05	1.20E-05	1.10E-05	1.10E-05
Am Gas Fraction	8.50E-11	2.60E-10	2.70E-11	5.50E-10	7.20E-13	3.20E-11
Ba(g)	2.90E-11	8.90E-11	5.40E-11	1.10E-09	2.10E-11	9.30E-10
Ba2(g)	2.90E-21	8.70E-21	1.70E-20	3.40E-19	4.00E-21	1.80E-19
BaBr(g)	9.20E-19	2.80E-18	1.00E-18	2.20E-17	2.60E-19	1.20E-17
BaBr2(g)	2.00E-26	6.10E-26	1.30E-26	3.10E-25	2.90E-27	1.50E-25
BaI(g)	2.60E-13	8.00E-13	7.50E-13	1.40E-11	3.30E-13	1.40E-11
BaI2(g)	2.50E-15	7.60E-15	1.20E-14	2.20E-13	9.30E-15	3.60E-13
Ba Gas	3.00E-11	9.00E-11	5.50E-11	1.10E-09	2.10E-11	9.50E-10
Ba	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.10E-03	1.10E-03
BaBr2	4.80E-18	4.90E-18	9.90E-18	1.20E-17	7.00E-17	7.90E-17
BaI2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.20E-06	5.40E-06
BaI2(l)	2.00E-07	2.00E-07	2.60E-06	2.30E-06	0.00E+00	0.00E+00
Ba(l)	9.10E-05	9.10E-05	4.40E-04	4.40E-04	0.00E+00	0.00E+00
BaTe	1.10E-12	1.10E-12	6.20E-13	6.20E-13	3.40E-13	3.40E-13
Ba Condensed	9.20E-05	9.20E-05	4.50E-04	4.50E-04	1.10E-03	1.10E-03
Ba Gas Fraction	3.20E-07	9.80E-07	1.20E-07	2.50E-06	2.00E-08	8.90E-07
Br(g)	6.90E-28	2.10E-27	1.30E-28	2.80E-27	5.20E-31	2.50E-29
Br2(g)	1.30E-47	3.90E-47	1.10E-48	2.50E-47	2.40E-52	1.20E-50
BaBr(g)	9.20E-19	2.80E-18	1.00E-18	2.20E-17	2.60E-19	1.20E-17
BaBr2(g)	2.00E-26	6.10E-26	1.30E-26	3.10E-25	2.90E-27	1.50E-25
CeBr3(g)	6.20E-43	1.90E-42	8.60E-44	2.20E-42	9.40E-46	5.20E-44
EuBr2(g)	7.40E-31	2.30E-30	6.90E-31	1.60E-29	3.80E-32	1.90E-30
IBr(g)	6.10E-39	1.90E-38	1.50E-39	3.00E-38	1.10E-42	5.10E-41
LaBr3(g)	5.80E-45	1.80E-44	7.50E-46	1.90E-44	7.70E-48	4.20E-46
MoBr(g)	3.10E-49	9.50E-49	3.00E-50	6.40E-49	2.00E-54	9.70E-53
MoBr2(g)	4.20E-59	1.30E-58	2.30E-60	5.50E-59	9.90E-65	5.10E-63

¹ The results listed in the table are moles per pin, unless noted as a fraction. The analysis includes only those radionuclides within the plenum region (and the “fraction” calculations are based on the fraction of the total amount of that radionuclide element in the plenum region). Species are assumed to be in the solid state, unless noted by (g) for gas, and (l) for liquid.

MoBr4(g)	5.60E-56	4.50E-46	2.70E-57	3.30E-47
MoBr5(g)	6.60E-71	9.00E-60	1.50E-72	3.00E-61
NaBr(g)	5.40E-09	1.20E-05	2.90E-09	1.20E-05
Na2Br2(g)	1.40E-13	1.00E-09	9.50E-14	1.70E-09
NbBr5(g)	7.70E-66	7.30E-54	2.40E-67	2.90E-55
NdBr3(g)	4.10E-28	1.90E-19	2.50E-28	1.80E-19
PdBr2(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00
PuBr3(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00
RbBr(g)	1.60E-10	4.00E-07	1.90E-10	6.50E-07
Rb2Br2(g)	4.70E-17	3.90E-13	1.50E-16	1.80E-12
SbBr3(g)	3.10E-42	2.20E-33	4.30E-43	4.70E-34
SeBr2(g)	1.80E-42	9.40E-36	3.40E-44	3.00E-37
Se2Br2(g)	3.70E-59	4.80E-51	8.30E-62	2.40E-53
SrBr(g)	6.90E-12	2.70E-07	9.10E-12	0.00E+00
SrBr2(g)	1.60E-16	1.00E-10	2.50E-16	3.20E-10
UBr(g)	4.90E-22	2.90E-14	6.00E-23	4.10E-15
UBr2(g)	5.00E-27	5.10E-18	7.00E-28	8.00E-19
UBr3(g)	7.20E-32	1.20E-21	1.20E-32	2.40E-22
UBr4(g)	1.80E-39	5.20E-28	2.70E-40	8.60E-29
UBr5(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ZrBr(g)	7.90E-26	1.30E-19	1.20E-26	3.20E-20
ZrBr2(g)	2.80E-30	7.80E-23	5.20E-31	2.30E-23
ZrBr3(g)	3.10E-32	1.50E-23	1.00E-32	7.30E-24
ZrBr4(g)	3.40E-41	2.70E-31	9.20E-42	1.10E-31
Br Gas	5.60E-09	1.40E-05	3.10E-09	1.40E-05
BaBr2	4.80E-11	2.00E-08	1.90E-10	5.80E-08
CeBr3	0.00E+00	0.00E+00	0.00E+00	0.00E+00
CsBr	3.70E-06	5.70E-07	8.90E-06	1.10E-06
EuBr2	1.20E-12	1.50E-10	3.90E-12	3.90E-10
LaBr3	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MoBr2	1.90E-30	5.60E-27	7.60E-31	2.10E-27
MoBr3	3.80E-43	1.90E-38	7.50E-44	3.50E-39
MoBr4	0.00E+00	0.00E+00	0.00E+00	0.00E+00
NaBr	6.50E-06	1.50E-06	7.00E-06	1.80E-06
NdBr3	1.50E-24	7.10E-20	2.00E-24	9.50E-20
NpBr3	0.00E+00	0.00E+00	0.00E+00	0.00E+00
NpBr4	0.00E+00	0.00E+00	0.00E+00	0.00E+00
PuBr3	0.00E+00	0.00E+00	0.00E+00	0.00E+00
RbBr	1.10E-07	2.80E-08	2.60E-07	5.50E-08
RhBr3	0.00E+00	0.00E+00	0.00E+00	0.00E+00
SrBr2	3.30E-11	2.20E-09	1.40E-10	1.20E-08
TeBr4	0.00E+00	0.00E+00	0.00E+00	0.00E+00
UBr3	3.90E-27	6.80E-21	1.80E-27	2.20E-21
UBr4	0.00E+00	0.00E+00	0.00E+00	0.00E+00
UBr5	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ZrBr2	2.30E-24	6.50E-21	1.60E-24	4.30E-21
ZrBr3	5.90E-33	2.90E-28	3.10E-33	1.40E-28
Br Condensed	1.00E-05	2.20E-06	1.60E-05	3.10E-06
Br Gas Fraction	5.50E-04	8.70E-01	1.90E-04	8.20E-01
Ce(g)	1.40E-15	1.30E-07	3.40E-16	3.90E-08
CeBr3(g)	1.60E-26	7.20E-15	9.50E-27	5.10E-15
CeI3(g)	9.90E-23	4.20E-13	1.60E-22	2.40E-13

MoBr3(g)	8.80E-75	2.80E-74	2.50E-76	6.30E-75	1.80E-81	9.70E-80
MoBr4(g)	1.70E-91	5.40E-91	2.30E-93	6.30E-92	2.30E-99	1.30E-97
MoBr5(g)	9.40E-115	3.00E-114	5.30E-117	1.60E-115	1.90E-124	1.20E-122
MoBr6(g)	4.40E-142	1.40E-141	9.00E-145	2.90E-143	4.10E-154	2.70E-152
NaBr(g)	1.00E-14	3.10E-14	2.90E-15	6.20E-14	2.60E-16	1.20E-14
Na2Br2(g)	2.40E-22	7.50E-22	4.30E-23	1.00E-21	4.60E-24	2.40E-22
NbBr5(g)	6.10E-103	2.00E-102	5.10E-105	1.50E-103	2.60E-111	1.60E-109
NbBr3O(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
NdBr3(g)	1.10E-45	3.50E-45	3.00E-46	7.70E-45	3.70E-48	2.00E-46
PdBr2(g)	1.10E-57	3.40E-57	1.50E-58	3.50E-57	1.10E-62	5.80E-61
PuBr3(g)	8.50E-43	2.70E-42	4.80E-44	1.20E-42	1.10E-46	5.90E-45
RbBr(g)	2.70E-16	8.20E-16	4.40E-16	9.10E-15	1.20E-16	5.90E-15
Rb2Br2(g)	2.40E-26	7.40E-26	1.40E-25	3.00E-24	1.10E-25	5.50E-24
SbBr3(g)	1.20E-65	3.80E-65	9.30E-67	2.40E-65	1.60E-71	8.70E-70
SeBr2(g)	7.20E-68	2.20E-67	1.10E-69	2.60E-68	1.60E-75	8.20E-74
Se2Br2(g)	1.00E-93	3.20E-93	2.40E-96	5.60E-95	6.60E-105	3.40E-103
SeOBr2(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
SrBr(g)	2.10E-19	6.40E-19	5.00E-19	1.10E-17	7.30E-20	3.50E-18
SrBr2(g)	1.30E-27	3.90E-27	1.90E-27	4.40E-26	2.40E-28	1.20E-26
UBr(g)	2.00E-34	6.00E-34	2.50E-35	5.30E-34	2.00E-38	9.70E-37
UBr2(g)	2.40E-43	7.30E-43	1.80E-44	4.10E-43	9.40E-48	4.80E-46
UBr3(g)	1.50E-51	4.60E-51	6.80E-53	1.70E-51	3.70E-56	2.00E-54
UBr4(g)	2.80E-64	8.70E-64	7.00E-66	1.90E-64	1.20E-69	6.90E-68
UBr5(g)	2.70E-87	8.60E-87	2.80E-89	8.30E-88	1.70E-94	1.10E-92
YBr2(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ZrBr(g)	2.70E-40	8.30E-40	7.30E-41	1.60E-39	4.50E-44	2.20E-42
ZrBr2(g)	2.30E-48	7.20E-48	3.90E-49	9.00E-48	2.00E-52	1.00E-50
ZrBr3(g)	3.80E-52	1.20E-51	4.50E-53	1.10E-51	6.50E-56	3.60E-54
ZrBr4(g)	1.90E-66	6.10E-66	1.20E-67	3.30E-66	4.60E-71	2.70E-69
Br Gas	1.00E-14	3.20E-14	3.30E-15	7.10E-14	3.80E-16	1.80E-14
BaBr2	4.80E-18	4.90E-18	9.90E-18	1.20E-17	7.00E-17	7.90E-17
CeBr3	2.40E-36	2.50E-36	8.90E-37	1.10E-36	1.90E-37	2.30E-37
CsBr	1.90E-10	1.90E-10	7.90E-10	7.80E-10	1.60E-09	1.50E-09
EuBr2	1.80E-20	1.90E-20	5.50E-20	6.40E-20	1.40E-19	1.60E-19
LaBr3	1.20E-38	1.20E-38	4.30E-39	5.50E-39	1.00E-39	1.20E-39
MoBr2	4.00E-49	4.10E-49	7.40E-50	8.70E-50	1.70E-52	1.90E-52
MoBr3	1.20E-69	1.30E-69	9.60E-71	1.20E-70	1.10E-74	1.40E-74
MoBr4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.40E-101	5.70E-101
NaBr	2.40E-10	2.50E-10	1.80E-10	1.90E-10	1.40E-10	1.50E-10
NdBr3	3.80E-40	3.90E-40	2.70E-40	3.50E-40	4.40E-41	5.30E-41
NpBr3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.40E-48	5.30E-48
NpBr4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.70E-73	8.60E-73
PuBr3	4.10E-37	4.30E-37	6.10E-38	7.70E-38	2.00E-39	2.40E-39
PuOBr	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
RbBr	2.20E-12	2.20E-12	8.90E-12	9.30E-12	1.60E-11	1.70E-11
RhBr3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.20E-78	2.60E-78
SrBr2	1.90E-19	1.90E-19	7.90E-19	9.30E-19	2.00E-18	2.30E-18
TeBr4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
UBr3	4.00E-44	4.10E-44	5.30E-45	6.60E-45	7.70E-47	9.30E-47
UBr4	4.30E-63	4.50E-63	2.50E-64	3.40E-64	1.50E-67	1.90E-67
UBr5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.60E-94	9.00E-94
ZrBr2	4.40E-38	4.50E-38	2.40E-38	2.80E-38	8.40E-40	9.50E-40
ZrBr3	1.30E-52	1.40E-52	3.60E-53	4.50E-53	2.40E-55	2.90E-55

CeSe(g)	2.70E-24	6.30E-15	2.10E-25	8.00E-16
CeTe(g)	8.60E-24	1.70E-14	7.40E-25	2.70E-15
Ce Gas	1.40E-15	1.30E-07	3.40E-16	3.90E-08
Ce	8.80E-05	0.00E+00	1.30E-04	0.00E+00
Ce(l)	2.60E-08	2.40E-04	4.00E-08	2.90E-04
CeBr3	0.00E+00	0.00E+00	0.00E+00	0.00E+00
CeI3	1.40E-19	5.90E-14	4.90E-19	4.70E-14
Ce Condensed	8.80E-05	2.40E-04	1.30E-04	2.90E-04
Ce Gas Fraction	1.60E-11	5.20E-04	2.50E-12	1.40E-04
Cs(g)	1.50E-04	1.40E-02	1.80E-04	2.10E-02
Cs2(g)	1.10E-06	1.20E-05	2.30E-06	3.50E-05
CsBr(g)	8.90E-09	1.40E-05	1.10E-08	2.30E-05
Cs2Br2(g)	5.30E-14	1.70E-10	1.90E-13	7.90E-10
CsI(g)	5.10E-07	1.60E-04	9.80E-07	2.80E-04
Cs2I2(g)	1.70E-10	2.60E-08	1.40E-09	1.20E-07
CsNa(g)	3.70E-05	6.30E-04	3.70E-05	1.20E-03
CsRb(g)	8.90E-08	1.60E-06	1.80E-07	4.70E-06
Cs Gas	1.90E-04	1.40E-02	2.20E-04	2.30E-02
CsBr	0.00E+00	0.00E+00	8.90E-06	1.10E-06
CsI(l)	6.20E-08	2.00E-09	1.80E-07	3.20E-09
Cs(l)	5.60E-03	5.10E-05	1.10E-02	8.60E-05
Cs2Te	1.10E-07	2.90E-09	2.90E-07	8.80E-09
Cs Condensed	5.60E-03	5.20E-05	1.10E-02	8.70E-05
Cs Gas Fraction	3.30E-02	1.00E+00	1.90E-02	1.00E+00
Eu(g)	2.80E-08	1.20E-04	2.30E-08	1.40E-04
EuBr2(g)	6.90E-19	8.90E-13	6.30E-19	1.00E-12
EuI3(g)	4.90E-27	1.00E-21	6.50E-27	4.90E-22
EuSe(g)	1.60E-19	1.80E-14	2.60E-20	5.00E-15
EuTe(g)	2.40E-18	2.30E-13	4.70E-19	8.70E-14
Eu Gas	2.80E-08	1.20E-04	2.30E-08	1.40E-04
Eu	0.00E+00	0.00E+00	0.00E+00	0.00E+00
EuBr2	1.20E-12	1.50E-10	3.90E-12	3.90E-10
EuI2	2.70E-10	1.60E-09	1.50E-09	3.10E-09
EuI3	2.70E-24	5.80E-23	8.40E-24	4.00E-23
EuSe	2.60E-06	3.00E-05	4.10E-06	4.90E-05
Eu(l)	7.50E-05	3.40E-05	1.50E-04	5.70E-05
EuTe	2.10E-05	2.10E-04	3.40E-05	4.00E-04
Eu Condensed	9.90E-05	2.80E-04	1.90E-04	5.00E-04
Eu Gas Fraction	2.80E-04	3.10E-01	1.20E-04	2.10E-01
I(g)	9.60E-14	2.40E-10	3.60E-14	8.20E-11
I2(g)	2.10E-23	1.90E-19	6.90E-24	3.60E-20
IBr(g)	6.10E-26	2.60E-21	1.10E-26	4.30E-22
IBa(g)	9.40E-11	4.90E-06	1.60E-10	6.30E-06
IBaI2(g)	1.40E-13	2.60E-08	4.10E-13	3.90E-08
IBr(g)	6.10E-26	2.60E-21	1.10E-26	4.30E-22
CeI3(g)	9.90E-23	4.20E-13	1.60E-22	2.40E-13
CsI(g)	5.10E-07	1.60E-04	9.80E-07	2.80E-04
Cs2I2(g)	1.70E-10	2.60E-08	1.40E-09	1.20E-07
EuI3(g)	4.90E-27	1.00E-21	6.50E-27	4.90E-22
LaI3(g)	5.50E-24	2.50E-17	9.70E-24	2.00E-17

ZrBr4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Br Condensed	4.40E-10	4.40E-10	9.80E-10	9.80E-10	1.70E-09	1.70E-09
Br Gas Fraction	2.40E-05	7.30E-05	3.40E-06	7.30E-05	2.20E-07	1.10E-05
Ce(g)	8.60E-23	2.60E-22	4.50E-23	9.10E-22	3.00E-25	1.30E-23
Ce2(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
CeBr3(g)	6.20E-43	1.90E-42	8.60E-44	2.20E-42	9.40E-46	5.20E-44
CeI3(g)	3.90E-27	1.20E-26	9.30E-27	1.60E-25	4.20E-28	1.50E-26
CeO(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
CeSe(g)	6.40E-36	1.90E-35	7.70E-37	1.50E-35	2.00E-40	9.10E-39
CeTe(g)	1.90E-35	5.70E-35	1.00E-36	2.00E-35	2.30E-40	1.10E-38
Ce Gas	8.60E-23	2.60E-22	4.50E-23	9.10E-22	3.00E-25	1.30E-23
Ce(l)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ce	2.40E-05	2.40E-05	4.80E-05	4.80E-05	7.10E-05	7.10E-05
CeBr3	2.40E-36	2.50E-36	8.90E-37	1.10E-36	1.90E-37	2.30E-37
CeI3	4.10E-22	4.10E-22	2.80E-21	2.40E-21	2.40E-21	1.90E-21
Ce Condensed	2.40E-05	2.40E-05	4.80E-05	4.80E-05	7.10E-05	7.10E-05
Ce Gas Fraction	3.70E-18	1.10E-17	9.30E-19	1.90E-17	4.20E-21	1.90E-19
Cs(g)	9.80E-06	2.90E-05	2.90E-05	5.20E-04	1.70E-05	7.40E-04
Cs2(g)	9.10E-09	2.60E-08	1.40E-07	2.30E-06	1.30E-07	5.10E-06
CsBr(g)	4.90E-14	1.50E-13	8.40E-14	1.70E-12	3.20E-14	1.40E-12
Cs2Br2(g)	1.60E-22	4.60E-22	9.70E-22	1.90E-20	1.10E-21	4.90E-20
CsI(g)	6.60E-08	1.90E-07	3.00E-07	5.20E-06	2.30E-07	9.00E-06
Cs2I2(g)	2.50E-10	7.30E-10	1.10E-08	1.70E-07	5.00E-08	1.70E-06
CsNa(g)	6.00E-07	1.80E-06	1.60E-06	2.90E-05	6.10E-07	2.60E-05
CsRb(g)	3.50E-10	1.00E-09	5.20E-09	9.20E-08	4.20E-09	1.80E-07
Cs2RuO4(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Cs Gas	1.10E-05	3.10E-05	3.10E-05	5.60E-04	1.90E-05	7.90E-04
Cs	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
CsBr	1.90E-10	1.90E-10	7.90E-10	7.80E-10	1.60E-09	1.50E-09
CsI(l)	4.50E-09	4.40E-09	4.50E-08	3.90E-08	7.90E-08	6.90E-08
Cs(l)	8.70E-04	8.50E-04	5.80E-03	5.30E-03	1.20E-02	1.10E-02
Cs2Te	3.30E-10	3.20E-10	1.60E-09	1.40E-09	2.30E-09	2.10E-09
Cs Condensed	8.70E-04	8.50E-04	5.80E-03	5.30E-03	1.20E-02	1.10E-02
Cs Gas Fraction	1.20E-02	3.50E-02	5.30E-03	9.60E-02	1.60E-03	6.80E-02
Eu(g)	1.10E-11	3.40E-11	3.10E-11	6.20E-10	5.90E-12	2.70E-10
EuBr2(g)	7.40E-31	2.30E-30	6.90E-31	1.60E-29	3.80E-32	1.90E-30
EuI3(g)	1.30E-34	3.90E-34	9.20E-34	1.60E-32	1.20E-35	4.50E-34
EuSe(g)	1.40E-29	4.20E-29	7.30E-30	1.50E-28	1.30E-32	6.00E-31
EuTe(g)	4.60E-28	1.40E-27	1.10E-28	2.20E-27	2.20E-31	1.00E-29
Eu Gas	1.10E-11	3.40E-11	3.10E-11	6.20E-10	5.90E-12	2.70E-10
Eu	8.80E-06	8.80E-06	6.60E-05	6.60E-05	1.40E-04	1.40E-04
EuBr2	1.80E-20	1.80E-20	5.50E-20	6.40E-20	1.40E-19	1.60E-19
EuBr3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
EuI2	7.70E-11	7.60E-11	1.40E-09	1.30E-09	5.60E-09	4.80E-09
EuI3	1.80E-29	1.80E-29	3.70E-28	3.20E-28	1.00E-28	8.10E-29
EuSe	1.20E-07	1.20E-07	3.00E-07	3.00E-07	4.80E-07	4.80E-07
Eu(l)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
EuTe	3.30E-07	3.30E-07	3.50E-07	3.50E-07	3.60E-07	3.60E-07
Eu Condensed	9.30E-06	9.30E-06	6.70E-05	6.70E-05	1.40E-04	1.40E-04
Eu Gas Fraction	1.20E-06	3.60E-06	4.60E-07	9.30E-06	4.10E-08	1.90E-06

Mol(g)	7.30E-28	2.60E-22	1.10E-28	4.00E-23
Mol2(g)	1.10E-31	1.40E-25	2.70E-32	2.40E-26
Mol3(g)	5.80E-41	2.60E-34	1.30E-41	2.70E-35
Mol4(g)	2.10E-51	3.50E-44	4.10E-52	2.00E-45
Mol5(g)	1.20E-65	7.20E-58	1.50E-66	1.70E-59
NaI(g)	3.40E-07	1.70E-04	2.70E-07	1.60E-04
Na2I2(g)	1.80E-10	6.20E-08	2.80E-10	9.70E-08
NbI2(g)	4.50E-29	3.90E-22	1.20E-29	6.40E-23
NbI3(g)	2.10E-37	6.80E-30	6.40E-38	7.90E-31
NbI4(g)	2.30E-48	2.60E-40	5.50E-49	1.60E-41
NbI5(g)	2.70E-58	1.10E-49	5.50E-59	3.80E-51
NdI3(g)	1.90E-24	8.50E-18	3.10E-24	6.30E-18
PuI3(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00
RbI(g)	1.00E-08	5.30E-06	1.90E-08	8.90E-06
Rb2I2(g)	9.30E-14	3.50E-11	6.60E-13	1.60E-10
SbI3(g)	1.10E-37	7.10E-31	4.40E-38	1.30E-31
SmI3(g)	1.00E-25	2.70E-18	1.70E-25	1.80E-18
SrI(g)	3.10E-10	2.50E-06	6.10E-10	6.60E-06
SrI2(g)	9.30E-14	2.80E-09	3.10E-13	8.00E-09
Tel2(g)	1.30E-29	2.70E-24	1.60E-30	2.70E-25
Tel4(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00
UI(g)	1.10E-21	1.40E-14	1.80E-22	1.70E-15
UI2(g)	1.40E-24	6.50E-17	4.00E-25	9.10E-18
UI3(g)	1.10E-28	1.80E-20	5.10E-29	2.70E-21
UI4(g)	1.80E-33	1.00E-24	9.50E-34	1.20E-25
YI3(g)	2.80E-26	8.90E-19	2.60E-26	3.20E-19
ZrI(g)	1.20E-25	4.10E-20	2.20E-26	8.20E-21
ZrI2(g)	7.70E-28	9.70E-22	2.90E-28	2.50E-22
ZrI3(g)	2.50E-28	1.10E-21	2.40E-28	4.90E-22
ZrI4(g)	3.10E-36	5.00E-29	3.50E-36	1.70E-29
I Gas	8.60E-07	3.40E-04	1.30E-06	4.60E-04
BaI2(l)	6.70E-08	1.30E-06	4.90E-07	2.90E-06
CeI3	1.40E-19	5.90E-14	4.90E-19	4.70E-14
CsI(l)	6.20E-08	2.00E-09	1.80E-07	3.20E-09
Eul2	2.70E-10	1.60E-09	1.50E-09	3.10E-09
Eul3	2.70E-24	5.80E-23	8.40E-24	4.00E-23
I2(l)	1.80E-22	1.60E-22	7.90E-23	2.70E-23
LaI3	5.50E-21	2.50E-18	2.10E-20	2.70E-18
Mol2	6.00E-26	7.80E-24	5.30E-26	2.90E-24
Mol3	1.00E-37	4.70E-35	6.60E-38	8.60E-36
Mol4	0.00E+00	0.00E+00	0.00E+00	0.00E+00
NaI(l)	1.20E-04	5.70E-06	1.70E-04	6.30E-06
NbI5	0.00E+00	0.00E+00	0.00E+00	0.00E+00
NdI3	2.10E-21	9.60E-19	7.30E-21	9.50E-19
PuI3	0.00E+00	0.00E+00	0.00E+00	0.00E+00
RbI(l)	4.40E-06	2.30E-07	1.50E-05	4.60E-07
SmI3	2.30E-23	6.20E-20	8.20E-23	5.70E-20
SrI2(l)	1.30E-08	4.00E-08	1.10E-07	1.70E-07
UI3	0.00E+00	0.00E+00	0.00E+00	0.00E+00
YI3	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ZrI2	1.50E-20	1.90E-18	2.10E-20	1.20E-18
ZrI3	1.20E-28	5.50E-26	1.80E-28	2.30E-26
I Condensed	1.20E-04	8.60E-06	1.90E-04	1.30E-05

I(g)	7.70E-19	2.30E-18	4.30E-19	8.20E-18	7.10E-21	3.00E-19
I2(g)	1.90E-31	5.80E-31	1.30E-31	2.30E-30	3.00E-34	1.20E-32
I3(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
IBr(g)	6.10E-39	1.90E-38	1.50E-39	3.00E-38	1.10E-42	5.10E-41
BaI(g)	2.60E-13	8.00E-13	7.50E-13	1.40E-11	3.30E-13	1.40E-11
BaI2(g)	2.50E-15	7.60E-15	1.20E-14	2.20E-13	9.30E-15	3.60E-13
IBr(g)	6.10E-39	1.90E-38	1.50E-39	3.00E-38	1.10E-42	5.10E-41
CeI3(g)	3.90E-27	1.20E-26	9.30E-27	1.60E-25	4.20E-28	1.50E-26
CsI(g)	6.60E-08	1.90E-07	3.00E-07	5.20E-06	2.30E-07	9.00E-06
Cs2I2(g)	2.50E-10	7.30E-10	1.10E-08	1.70E-07	5.00E-08	1.70E-06
Eul3(g)	1.30E-34	3.90E-34	9.20E-34	1.60E-32	1.20E-35	4.50E-34
LaI3(g)	7.50E-29	2.20E-28	1.60E-28	2.90E-27	7.40E-30	2.70E-28
Mol(g)	2.40E-42	7.30E-42	6.20E-43	1.20E-41	1.00E-46	4.20E-45
Mol2(g)	9.30E-46	2.80E-45	3.80E-46	6.90E-45	8.30E-50	3.30E-48
Mol3(g)	1.60E-57	4.80E-57	8.10E-58	1.40E-56	3.60E-62	1.30E-60
Mol4(g)	8.30E-71	2.50E-70	5.00E-71	8.40E-70	3.40E-76	1.20E-74
Mol5(g)	1.90E-89	5.80E-89	1.20E-89	2.00E-88	4.70E-96	1.50E-94
Mol6(g)	7.30E-112	2.20E-111	4.30E-112	6.60E-111	3.40E-120	9.90E-119
NaI(g)	1.60E-08	4.80E-08	1.20E-08	2.30E-07	2.20E-09	9.40E-08
Na2I2(g)	9.70E-11	2.90E-10	1.20E-10	2.20E-09	4.50E-11	1.70E-09
NbI2(g)	1.70E-37	5.10E-37	9.30E-38	1.70E-36	1.40E-40	5.50E-39
NbI3(g)	1.70E-47	5.10E-47	1.20E-47	2.20E-46	6.40E-51	2.30E-49
NbI4(g)	1.20E-61	3.70E-61	1.10E-61	1.80E-60	7.00E-66	2.40E-64
NbI5(g)	1.60E-74	4.70E-74	1.60E-74	2.50E-73	1.50E-79	4.70E-78
NdI3(g)	4.40E-30	1.30E-29	2.00E-29	3.60E-28	9.70E-31	3.50E-29
PuI3(g)	5.40E-26	1.60E-25	5.50E-26	9.60E-25	8.40E-28	3.00E-26
RbI(g)	4.30E-10	1.30E-09	1.80E-09	3.40E-08	1.10E-09	4.60E-08
Rb2I2(g)	1.80E-14	5.40E-14	7.10E-13	1.20E-11	2.10E-12	8.10E-11
SbI3(g)	1.10E-48	3.40E-48	1.50E-48	2.70E-47	1.40E-52	5.20E-51
SmI3(g)	1.00E-30	3.10E-30	3.10E-30	5.40E-29	1.10E-31	4.10E-30
SrI(g)	1.90E-13	5.60E-13	1.20E-12	2.30E-11	3.40E-13	1.40E-11
SrI2(g)	1.60E-16	4.90E-16	1.60E-15	3.00E-14	6.60E-16	2.60E-14
Tel2(g)	9.40E-42	2.80E-41	6.50E-43	1.20E-41	7.30E-47	2.80E-45
Tel4(g)	3.00E-83	9.10E-83	2.00E-84	3.30E-83	1.90E-91	6.40E-90
UI(g)	1.90E-30	5.70E-30	5.80E-31	1.10E-29	5.90E-34	2.50E-32
UI2(g)	9.30E-33	2.80E-32	4.60E-33	8.50E-32	6.90E-36	2.70E-34
UI3(g)	1.70E-36	5.10E-36	1.30E-36	2.30E-35	2.70E-39	9.70E-38
UI4(g)	1.30E-42	4.00E-42	1.40E-42	2.40E-41	1.40E-45	4.70E-44
YI2(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
YI3(g)	1.10E-30	3.20E-30	2.40E-30	4.20E-29	7.80E-32	2.80E-30
ZrI(g)	8.30E-37	2.50E-36	5.40E-37	1.00E-35	3.40E-40	1.40E-38
ZrI2(g)	8.50E-38	2.60E-37	9.40E-38	1.70E-36	1.40E-40	5.30E-39
ZrI3(g)	6.20E-36	1.90E-35	1.30E-35	2.30E-34	9.20E-38	3.40E-36
ZrI4(g)	3.80E-45	1.20E-44	1.10E-44	1.80E-43	3.40E-47	1.10E-45
I Gas	8.30E-08	2.40E-07	3.40E-07	5.80E-06	3.30E-07	1.30E-05
BaI2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.20E-06	5.40E-06
BaI2(l)	2.00E-07	2.00E-07	2.60E-06	2.30E-06	0.00E+00	0.00E+00
CeI3	4.10E-22	4.10E-22	2.80E-21	2.40E-21	2.40E-21	1.90E-21
CsI	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
CsI(l)	4.50E-09	4.40E-09	4.50E-08	3.90E-08	7.90E-08	6.90E-08
Eul2	7.70E-11	7.60E-11	1.40E-09	1.30E-09	5.60E-09	4.80E-09
Eul3	1.80E-29	1.80E-29	3.70E-28	3.20E-28	1.00E-28	8.10E-29

I Gas Fraction	7.10E-03	9.80E-01	6.80E-03	9.70E-01
La(g)	2.00E-17	2.00E-12	5.20E-18	8.20E-13
LaBr3(g)	5.70E-28	2.70E-19	3.50E-28	2.60E-19
LaI3(g)	5.50E-24	2.50E-17	9.70E-24	2.00E-17
LaSe(g)	3.60E-24	9.00E-18	3.30E-25	1.70E-18
LaTe(g)	7.10E-24	1.50E-17	7.10E-25	3.50E-18
La Gas	2.00E-17	2.00E-12	5.20E-18	8.20E-13
La	2.00E-06	2.00E-05	3.30E-06	3.30E-05
La(l)	2.00E-06	2.00E-05	3.30E-06	3.30E-05
LaBr3	0.00E+00	0.00E+00	0.00E+00	0.00E+00
LaTe	1.50E-10	3.20E-08	1.30E-10	4.10E-08
La2Te3	5.80E-27	8.20E-20	1.70E-27	9.00E-20
La Condensed	4.10E-06	4.10E-05	6.50E-06	6.50E-05
La Gas Fraction	5.00E-12	4.90E-08	8.00E-13	1.30E-08
Mo(g)	6.00E-23	5.90E-18	6.80E-24	1.10E-18
Mo2(g)	4.10E-34	5.60E-27	3.00E-35	7.90E-28
MoBr(g)	3.80E-30	6.30E-24	3.50E-31	9.10E-25
MoBr2(g)	6.00E-36	1.70E-28	5.90E-37	2.60E-29
MoBr3(g)	1.30E-45	6.30E-37	9.60E-47	7.00E-38
MoBr4(g)	5.60E-56	4.50E-46	2.70E-57	3.30E-47
Mol(g)	7.30E-28	2.60E-22	1.10E-28	4.00E-23
Mol2(g)	1.10E-31	1.40E-25	2.70E-32	2.40E-26
Mol3(g)	5.80E-41	2.60E-34	1.30E-41	2.70E-35
Mol4(g)	2.10E-51	3.50E-44	4.10E-52	2.00E-45
Mo Gas	6.00E-23	5.90E-18	6.80E-24	1.10E-18
Mo	1.20E-05	1.20E-04	2.00E-05	2.00E-04
Mo(l)	3.10E-06	3.10E-05	4.50E-06	4.50E-05
MoBr2	1.90E-30	5.60E-27	7.60E-31	2.10E-27
MoBr3	3.80E-43	1.90E-38	7.50E-44	3.50E-39
MoBr4	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Mol2	6.00E-26	7.80E-24	5.30E-26	2.90E-24
Mol3	1.00E-37	4.70E-35	6.60E-38	8.60E-36
Mol4	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MoSe2	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Mo3Se4	3.10E-69	2.50E-58	1.70E-71	5.30E-60
Mo2	3.20E-12	4.50E-09	2.30E-12	3.80E-09
MoTe2	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Mo Condensed	1.50E-05	1.50E-04	2.50E-05	2.50E-04
Mo Gas Fraction	4.00E-18	3.90E-14	2.70E-19	4.30E-15
Na(g)	1.90E-03	2.60E-01	1.00E-03	2.50E-01
Na2(g)	4.00E-04	1.00E-02	1.90E-04	1.20E-02
NaBr(g)	5.40E-09	1.20E-05	2.90E-09	1.20E-05
Na2Br2(g)	1.40E-13	1.00E-09	9.50E-14	1.70E-09
NaI(g)	3.40E-07	1.70E-04	2.70E-07	1.60E-04
Na2I2(g)	1.80E-10	6.20E-08	2.80E-10	9.70E-08
RbNa(g)	1.40E-06	3.90E-05	1.40E-06	7.10E-05
CsNa(g)	3.70E-05	6.30E-04	3.70E-05	1.20E-03
Na Gas	2.70E-03	2.80E-01	1.40E-03	2.80E-01
NaBr	6.50E-06	1.50E-06	7.00E-06	1.80E-06
NaI(l)	1.20E-04	5.70E-06	1.70E-04	6.30E-06

I2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
I2(l)	4.80E-31	4.80E-31	6.90E-31	6.20E-31	3.20E-33	2.70E-33
LaI3	4.60E-24	4.60E-24	2.90E-23	2.50E-23	2.40E-23	1.90E-23
Mol2	5.70E-36	5.70E-36	7.40E-36	6.70E-36	6.60E-38	5.70E-38
Mol3	2.60E-51	2.60E-51	3.80E-51	3.30E-51	3.30E-54	2.70E-54
Mol4	2.30E-66	2.30E-66	3.60E-66	3.00E-66	2.40E-70	1.80E-70
Mol5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
NaI	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.50E-05	6.00E-05
NaI(l)	3.60E-05	3.60E-05	6.60E-05	6.20E-05	0.00E+00	0.00E+00
NbI5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
NdI3	2.80E-25	2.80E-25	3.60E-24	3.20E-24	2.60E-24	2.10E-24
NpI3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.10E-30	8.40E-31
PdI2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
PuI3	2.70E-21	2.70E-21	7.40E-21	6.50E-21	1.60E-21	1.20E-21
RbI	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
RbI(l)	1.90E-06	1.90E-06	2.00E-05	1.80E-05	6.40E-05	5.80E-05
RbI3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
RuI3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
SbI3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.40E-53	1.10E-53
SbSeI	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
SmI3	2.60E-26	2.60E-26	2.20E-25	1.90E-25	1.40E-25	1.10E-25
SrI2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
SrI2(l)	3.40E-09	3.40E-09	9.40E-08	8.60E-08	4.70E-07	4.00E-07
Tel4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
UI3	4.60E-29	4.60E-29	1.10E-28	9.40E-29	5.50E-30	4.40E-30
YI3	5.70E-26	5.70E-26	3.60E-25	3.10E-25	1.90E-25	1.50E-25
ZrI	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ZrI2	5.20E-26	5.20E-26	2.00E-25	1.80E-25	2.00E-26	1.80E-26
ZrI3	3.70E-36	3.70E-36	1.70E-35	1.50E-35	5.20E-37	4.20E-37
I Condensed	3.90E-05	3.90E-05	9.10E-05	8.60E-05	1.40E-04	1.30E-04
I Gas Fraction	2.10E-03	6.30E-03	3.70E-03	6.40E-02	2.30E-03	8.80E-02
La(g)	2.90E-25	8.70E-25	1.40E-25	2.80E-24	8.00E-28	3.60E-26
La2(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
LaBr3(g)	5.80E-45	1.80E-44	7.50E-46	1.90E-44	7.70E-48	4.20E-46
LaI3(g)	7.50E-29	2.20E-28	1.60E-28	2.90E-27	7.40E-30	2.70E-28
LaSe(g)	8.60E-36	2.60E-35	1.00E-36	2.00E-35	3.70E-40	1.70E-38
LaTe(g)	1.20E-35	3.70E-35	6.30E-37	1.30E-35	1.90E-40	8.50E-39
La Gas	2.90E-25	8.70E-25	1.40E-25	2.80E-24	8.00E-28	3.60E-26
La(l)	1.20E-07	1.20E-07	2.30E-07	2.30E-07	2.70E-07	2.70E-07
La	1.40E-07	1.40E-07	2.70E-07	2.70E-07	3.60E-07	3.60E-07
LaBr3	1.20E-38	1.20E-38	4.30E-39	5.50E-39	1.00E-39	1.20E-39
LaTe	7.80E-14	7.80E-14	1.80E-14	1.80E-14	4.10E-15	4.10E-15
La2Te3	4.70E-37	4.70E-37	2.20E-39	2.30E-39	7.10E-42	7.10E-42
La Condensed	2.70E-07	2.70E-07	5.00E-07	5.00E-07	6.30E-07	6.30E-07
La Gas Fraction	1.10E-18	3.30E-18	2.80E-19	5.60E-18	1.30E-21	5.80E-20
Mo(g)	1.60E-36	4.70E-36	2.80E-37	5.70E-36	8.20E-41	3.70E-39
Mo2(g)	1.70E-54	5.30E-54	1.80E-55	3.70E-54	2.90E-60	1.30E-58
MoBr(g)	3.10E-49	9.50E-49	3.00E-50	6.40E-49	2.00E-54	9.70E-53
MoBr2(g)	4.20E-59	1.30E-58	2.30E-60	5.50E-59	9.90E-65	5.10E-63
MoBr3(g)	8.80E-75	2.80E-74	2.50E-76	6.30E-75	1.80E-81	9.70E-80
MoBr4(g)	1.70E-91	5.40E-91	2.30E-93	6.30E-92	2.30E-99	1.30E-97

Na(l)	2.40E-01	3.30E-03	2.50E-01	3.90E-03
NaTe(l)	0.00E+00	0.00E+00	0.00E+00	0.00E+00
NaTe3	0.00E+00	0.00E+00	0.00E+00	0.00E+00
NaTe3(l)	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Na2Te	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Na Condensed	2.40E-01	3.30E-03	2.50E-01	3.90E-03
Na Gas Fraction	1.10E-02	9.90E-01	5.60E-03	9.90E-01
Nb(g)	7.80E-27	5.30E-21	4.20E-28	3.90E-22
NbBr5(g)	7.70E-66	7.30E-54	2.40E-67	2.90E-55
NbI2(g)	4.50E-29	3.90E-22	1.20E-29	6.40E-23
NbI3(g)	2.10E-37	6.80E-30	6.40E-38	7.90E-31
NbI4(g)	2.30E-48	2.60E-40	5.50E-49	1.60E-41
NbI5(g)	2.70E-58	1.10E-49	5.50E-59	3.80E-51
Nb Gas	7.80E-27	5.70E-21	4.30E-28	4.60E-22
Nb	1.40E-07	1.00E-05	1.50E-07	8.90E-06
Nb(l)	6.00E-08	4.20E-06	5.70E-08	3.40E-06
Nb Condensed	2.00E-07	1.40E-05	2.00E-07	1.20E-05
Nb Gas Fraction	3.80E-20	4.00E-16	2.10E-21	3.70E-17
Nd(g)	2.60E-14	2.50E-09	1.00E-14	1.60E-09
NdBr3(g)	4.10E-28	1.90E-19	2.50E-28	1.80E-19
NdI3(g)	1.90E-24	8.50E-18	3.10E-24	6.30E-18
NdSe(g)	7.40E-24	1.80E-17	7.40E-25	3.80E-18
NdTe(g)	5.60E-23	1.20E-16	6.40E-24	3.20E-17
Nd Gas	2.60E-14	2.50E-09	1.00E-14	1.60E-09
Nd	5.40E-06	5.40E-05	8.90E-06	8.90E-05
Nd(l)	5.40E-06	5.40E-05	8.90E-06	8.90E-05
NdI3	2.10E-21	9.60E-19	7.30E-21	9.50E-19
NdSe	1.20E-11	3.10E-09	1.10E-11	3.70E-09
Nd2Se3	3.10E-30	7.00E-23	7.70E-31	4.50E-23
Nd Condensed	5.40E-06	5.40E-05	8.90E-06	8.90E-05
Nd Gas Fraction	4.80E-09	4.70E-05	1.10E-09	1.80E-05
Np(g)	7.60E-19	7.40E-14	1.10E-19	1.20E-14
Np Gas	7.60E-19	7.40E-14	1.10E-19	1.20E-14
Np	7.80E-07	7.80E-06	7.60E-07	5.30E-06
Np(l)	7.80E-07	7.80E-06	7.60E-07	5.30E-06
NpBr3	0.00E+00	0.00E+00	0.00E+00	0.00E+00
NpBr4	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Np Condensed	1.60E-06	1.60E-05	1.50E-06	1.10E-05
Np Gas Fraction	4.90E-13	4.80E-09	7.10E-14	1.10E-09
Pd(g)	2.70E-15	2.70E-10	8.90E-16	1.40E-10
PdBr2(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Pd Gas	2.70E-15	2.70E-10	8.90E-16	1.40E-10
Pd	5.50E-06	5.50E-05	9.50E-06	9.50E-05
Pd(l)	4.60E-06	4.60E-05	7.60E-06	7.60E-05
PdTe	0.00E+00	0.00E+00	0.00E+00	0.00E+00
PdTe2	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Pd Condensed	1.00E-05	1.00E-04	1.70E-05	1.70E-04
Pd Gas Fraction	2.70E-10	2.60E-06	5.20E-11	8.20E-07

MoBr5(g)	9.40E-115	3.00E-114	5.30E-117	1.60E-115	1.90E-124	1.20E-122
MoBr6(g)	4.40E-142	1.40E-141	9.00E-145	2.90E-143	4.10E-154	2.70E-152
Mol(g)	2.40E-42	7.30E-42	6.20E-43	1.20E-41	1.00E-46	4.20E-45
Mol2(g)	9.30E-46	2.80E-45	3.80E-46	6.90E-45	8.30E-50	3.30E-48
Mol3(g)	1.60E-57	4.80E-57	8.10E-58	1.40E-56	3.60E-62	1.30E-60
Mol4(g)	8.30E-71	2.50E-70	5.00E-71	8.40E-70	3.40E-76	1.20E-74
Mol5(g)	1.90E-89	5.80E-89	1.20E-89	2.00E-88	4.70E-96	1.50E-94
Mol6(g)	7.30E-112	2.20E-111	4.30E-112	6.60E-111	3.40E-120	9.90E-119
BaMoO4(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Mo Gas	1.60E-36	4.70E-36	2.80E-37	5.70E-36	8.20E-41	3.70E-39
Mo(l)	1.40E-09	1.40E-09	1.40E-09	1.40E-09	9.60E-10	9.60E-10
Mo	2.20E-08	2.20E-08	2.30E-08	2.30E-08	2.30E-08	2.30E-08
MoBr2	4.00E-49	4.10E-49	7.40E-50	8.70E-50	1.70E-52	1.90E-52
MoBr3	1.20E-69	1.30E-69	9.60E-71	1.20E-70	1.10E-74	1.40E-74
MoBr4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.40E-101	5.70E-101
Mol2	5.70E-36	5.70E-36	7.40E-36	6.70E-36	6.60E-38	5.70E-38
Mol3	2.60E-51	2.60E-51	3.80E-51	3.30E-51	3.30E-54	2.70E-54
Mol4	2.30E-66	2.30E-66	3.60E-66	3.00E-66	2.40E-70	1.80E-70
MoSe2	2.40E-50	2.40E-50	8.50E-52	8.50E-52	5.90E-56	5.90E-56
Mo3Se4	2.50E-104	2.50E-104	2.20E-107	2.30E-107	1.30E-115	1.30E-115
Mo2	8.60E-24	8.60E-24	4.20E-24	4.20E-24	5.80E-26	5.80E-26
MoTe2	6.20E-46	6.20E-46	4.50E-48	4.50E-48	3.30E-52	3.30E-52
Mo3Te4	6.50E-97	6.50E-97	2.30E-101	2.40E-101	1.50E-109	1.60E-109
Mo Condensed	2.40E-08	2.40E-08	2.40E-08	2.40E-08	2.40E-08	2.40E-08
Mo Gas Fraction	6.60E-29	2.00E-28	1.20E-29	2.40E-28	3.50E-33	1.60E-31
Na(g)	1.50E-04	4.50E-04	7.60E-05	1.50E-03	1.60E-05	7.30E-04
Na2(g)	1.40E-05	4.20E-05	6.50E-06	1.30E-04	1.00E-06	4.60E-05
NaBr(g)	1.00E-14	3.10E-14	2.90E-15	6.20E-14	2.60E-16	1.20E-14
Na2Br2(g)	2.40E-22	7.50E-22	4.30E-23	1.00E-21	4.60E-24	2.40E-22
NaI(g)	1.60E-08	4.80E-08	1.20E-08	2.30E-07	2.20E-09	9.40E-08
Na2I2(g)	9.70E-11	2.90E-10	1.20E-10	2.20E-09	4.50E-11	1.70E-09
RbNa(g)	1.00E-08	3.00E-08	2.60E-08	5.10E-07	8.40E-09	3.80E-07
CsNa(g)	6.00E-07	1.80E-06	1.60E-06	2.90E-05	6.10E-07	2.60E-05
Na Gas	1.80E-04	5.40E-04	8.90E-05	1.80E-03	1.80E-05	8.30E-04
Na	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
NaBr	2.40E-10	2.50E-10	1.80E-10	1.90E-10	1.40E-10	1.50E-10
NaBrO3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
NaI	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.50E-05	6.00E-05
NaI(l)	3.60E-05	3.60E-05	6.60E-05	6.20E-05	0.00E+00	0.00E+00
Na(l)	2.00E-01	2.00E-01	2.40E-01	2.40E-01	2.50E-01	2.50E-01
NaSb	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Na3Sb	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
NaTe	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
NaTe(l)	4.00E-27	4.00E-27	3.80E-28	3.70E-28	1.70E-30	1.70E-30
NaTe3	1.20E-59	1.20E-59	8.30E-63	8.30E-63	5.00E-69	5.00E-69
NaTe3(l)	9.80E-73	9.80E-73	5.70E-76	5.70E-76	7.40E-83	7.40E-83
Na2Te	8.10E-24	8.10E-24	8.20E-25	8.10E-25	7.80E-27	7.80E-27
Na2Te(l)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Na2Te2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Na Condensed	2.00E-01	2.00E-01	2.40E-01	2.40E-01	2.50E-01	2.50E-01
Na Gas Fraction	9.00E-04	2.70E-03	3.70E-04	7.40E-03	7.20E-05	3.20E-03

Pu(g)	1.30E-13	9.80E-06	2.60E-14	2.30E-06
PuBr3(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00
PuI3(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Pu Gas	1.30E-13	9.80E-06	2.60E-14	2.30E-06
Pu	2.30E-04	0.00E+00	2.20E-04	0.00E+00
Pu(l)	2.90E-07	2.30E-03	2.80E-07	1.60E-03
PuBr3	0.00E+00	0.00E+00	0.00E+00	0.00E+00
PuI3	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Pu Condensed	2.30E-04	2.30E-03	2.20E-04	1.60E-03
Pu Gas Fraction	5.40E-10	4.20E-03	1.20E-10	1.50E-03
Rb(g)	7.10E-06	1.00E-03	7.90E-06	1.60E-03
Rb2(g)	2.10E-09	6.00E-08	4.10E-09	1.80E-07
RbBr(g)	1.60E-10	4.00E-07	1.90E-10	6.50E-07
Rb2Br2(g)	4.70E-17	3.90E-13	1.50E-16	1.80E-12
RbI(g)	1.00E-08	5.30E-06	1.90E-08	8.90E-06
Rb2I2(g)	9.30E-14	3.50E-11	6.60E-13	1.60E-10
RbNa(g)	1.40E-06	3.90E-05	1.40E-06	7.10E-05
CsRb(g)	8.90E-08	1.60E-06	1.80E-07	4.70E-06
Rb Gas	8.50E-06	1.10E-03	9.30E-06	1.70E-03
RbBr	1.10E-07	2.80E-08	2.60E-07	5.50E-08
RbI(l)	0.00E+00	0.00E+00	1.50E-05	4.60E-07
Rb(l)	4.40E-06	2.30E-07	8.30E-04	1.10E-05
Rb Condensed	4.20E-04	6.30E-06	8.40E-04	1.10E-05
Rb Gas Fraction	2.00E-02	9.90E-01	1.10E-02	9.90E-01
Rh(g)	3.90E-20	3.90E-15	6.30E-21	9.90E-16
Rh Gas	3.90E-20	3.90E-15	6.30E-21	9.90E-16
Rh	2.70E-06	2.70E-05	4.40E-06	4.40E-05
Rh(l)	1.60E-06	1.60E-05	2.40E-06	2.40E-05
RhBr3	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Rh3U	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Rh Condensed	4.30E-06	4.30E-05	6.80E-06	6.80E-05
Rh Gas Fraction	9.20E-15	9.00E-11	9.20E-16	1.50E-11
Ru(g)	6.20E-22	5.80E-18	6.80E-23	6.00E-19
Ru Gas	6.20E-22	5.80E-18	6.80E-23	6.00E-19
Ru	1.50E-05	1.50E-05	2.40E-05	1.30E-05
RuSe2	7.40E-34	4.60E-31	4.30E-35	2.60E-32
Ru Condensed	1.50E-05	1.50E-05	2.40E-05	1.30E-05
Ru Gas Fraction	4.00E-17	4.00E-13	2.90E-18	4.50E-14
Sb(g)	1.50E-12	2.20E-07	6.90E-13	1.60E-07
Sb2(g)	1.20E-16	3.60E-09	9.30E-17	5.40E-09
Sb3(g)	9.90E-23	6.10E-13	9.50E-23	1.40E-12
Sb4(g)	9.00E-28	1.20E-15	1.70E-27	5.90E-15
SbBr3(g)	3.10E-42	2.20E-33	4.30E-43	4.70E-34
SbI3(g)	1.10E-37	7.10E-31	4.40E-38	1.30E-31
SbSe(g)	1.30E-24	4.90E-18	1.10E-25	8.90E-19
SbTe(g)	2.20E-22	7.00E-16	2.50E-23	1.90E-16
Sb Gas	1.50E-12	2.30E-07	6.90E-13	1.70E-07
Sb	7.20E-07	1.10E-05	1.10E-06	1.60E-05
Sb2Se3	2.00E-55	1.00E-47	1.50E-57	2.00E-49

Nb(g)	7.10E-39	2.20E-38	1.20E-39	2.50E-38	1.60E-43	7.30E-42
NbBr5(g)	6.10E-103	2.00E-102	5.10E-105	1.50E-103	2.60E-111	1.60E-109
NbBr3O(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
NbI2(g)	1.70E-37	5.10E-37	9.30E-38	1.70E-36	1.40E-40	5.50E-39
NbI3(g)	1.70E-47	5.10E-47	1.20E-47	2.20E-46	6.40E-51	2.30E-49
NbI4(g)	1.20E-61	3.70E-61	1.10E-61	1.80E-60	7.00E-66	2.40E-64
NbI5(g)	1.60E-74	4.70E-74	1.60E-74	2.50E-73	1.50E-79	4.70E-78
NbO(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
NbO2(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
NbOI3(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Nb Gas	1.80E-37	5.30E-37	9.40E-38	1.70E-36	1.40E-40	5.60E-39
Nb(l)	3.10E-08	3.10E-08	3.20E-08	3.20E-08	2.80E-08	2.80E-08
Nb	1.60E-07	1.60E-07	1.70E-07	1.70E-07	1.80E-07	1.80E-07
Nb Condensed	1.90E-07	1.90E-07	2.00E-07	2.00E-07	2.00E-07	2.00E-07
Nb Gas Fraction	9.20E-31	2.80E-30	4.60E-31	8.50E-30	6.90E-34	2.70E-32
Nd(g)	1.50E-20	4.50E-20	1.80E-20	3.60E-19	5.20E-22	2.40E-20
NdBr3(g)	1.10E-45	3.50E-45	3.00E-46	7.70E-45	3.70E-48	2.00E-46
NdI3(g)	4.40E-30	1.30E-29	2.00E-29	3.60E-28	9.70E-31	3.50E-29
NdO(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
NdSe(g)	1.50E-35	4.50E-35	3.90E-36	7.80E-35	2.30E-39	1.10E-37
NdTe(g)	1.60E-34	4.80E-34	1.80E-35	3.70E-34	1.10E-38	4.90E-37
Nd Gas	1.50E-20	4.50E-20	1.80E-20	3.60E-19	5.20E-22	2.40E-20
Nd(l)	1.90E-07	1.90E-07	7.70E-07	7.70E-07	1.40E-06	1.40E-06
Nd	2.30E-07	2.30E-07	9.50E-07	9.50E-07	1.90E-06	1.90E-06
NdI3	2.80E-25	2.80E-25	3.60E-24	3.20E-24	2.60E-24	2.10E-24
NdSe	1.10E-14	1.10E-14	1.30E-14	1.30E-14	6.70E-15	6.70E-15
Nd2Se3	1.10E-40	1.10E-40	3.00E-41	3.00E-41	3.00E-43	3.00E-43
Nd Condensed	4.10E-07	4.10E-07	1.70E-06	1.70E-06	3.30E-06	3.30E-06
Nd Gas Fraction	3.60E-14	1.10E-13	1.10E-14	2.10E-13	1.60E-16	7.20E-15
Np(g)	6.00E-26	1.80E-25	1.50E-26	2.90E-25	4.90E-29	2.20E-27
NpO(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Np Gas	6.00E-26	1.80E-25	1.50E-26	2.90E-25	4.90E-29	2.20E-27
Np(l)	7.70E-07	7.70E-07	7.50E-07	7.50E-07	7.40E-07	7.40E-07
Np	7.70E-07	7.70E-07	7.50E-07	7.50E-07	7.40E-07	7.40E-07
NpBr3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.40E-48	5.30E-48
NpBr4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.70E-73	8.60E-73
NpOBr2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
NpI3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.10E-30	8.40E-31
NpI3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.10E-30	8.40E-31
NpO2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Np Condensed	7.70E-07	7.70E-07	7.50E-07	7.50E-07	7.40E-07	7.40E-07
Np Gas Fraction	7.90E-20	2.40E-19	1.90E-20	3.90E-19	6.60E-23	3.00E-21
Pd(g)	4.10E-22	1.20E-21	2.70E-22	5.30E-21	3.30E-24	1.50E-22
PdBr2(g)	1.10E-57	3.40E-57	1.50E-58	3.50E-57	1.10E-62	5.80E-61
PdO(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Pd Gas	4.10E-22	1.20E-21	2.70E-22	5.30E-21	3.30E-24	1.50E-22
Pd(l)	3.10E-07	3.10E-07	7.30E-07	7.30E-07	1.00E-06	1.00E-06
Pd	6.10E-07	6.10E-07	1.50E-06	1.50E-06	2.30E-06	2.30E-06
PdTe	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.60E-28	4.60E-28
PdTe2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.40E-51	4.40E-51

Sb(l)	6.70E-07	9.90E-06	9.90E-07	1.50E-05
Sb2Te3	8.30E-48	2.60E-40	9.90E-50	1.20E-41
USb2	0.00E+00	0.00E+00	0.00E+00	0.00E+00
U3Sb4	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Sb Condensed	1.40E-06	2.10E-05	2.10E-06	3.10E-05
Sb Gas Fraction	1.10E-06	1.10E-02	3.40E-07	5.60E-03
Se(g)	3.40E-21	6.10E-17	1.70E-22	5.30E-18
Se2(g)	2.70E-33	1.20E-27	2.80E-35	2.80E-29
Se3(g)	2.10E-49	2.50E-42	2.80E-52	9.40E-45
Se4(g)	1.50E-64	4.40E-56	2.70E-68	3.00E-59
SeBr2(g)	1.80E-42	9.40E-36	3.40E-44	3.00E-37
Se2Br2(g)	3.70E-59	4.80E-51	8.30E-62	2.40E-53
SeTe(g)	1.00E-30	3.90E-25	1.30E-32	1.30E-26
EuSe(g)	1.60E-19	1.80E-14	2.60E-20	5.00E-15
LaSe(g)	3.60E-24	9.00E-18	3.30E-25	1.70E-18
NdSe(g)	7.40E-24	1.80E-17	7.40E-25	3.80E-18
SbSe(g)	1.30E-24	4.90E-18	1.10E-25	8.90E-19
SmSe(g)	1.10E-22	1.70E-15	1.50E-23	4.10E-16
SrSe(g)	1.60E-19	9.60E-15	3.90E-20	5.80E-15
USe(g)	6.00E-27	5.30E-19	1.80E-28	2.40E-20
USe2(g)	5.40E-38	1.20E-28	4.20E-40	1.80E-30
YSe(g)	2.40E-26	4.20E-19	1.20E-27	3.80E-20
Se Gas	3.40E-21	6.10E-17	1.70E-22	5.30E-18
EuSe	2.60E-06	3.00E-05	4.10E-06	4.90E-05
LaSe	1.10E-11	2.80E-09	9.90E-12	3.20E-09
La2Se3	6.50E-31	1.50E-23	1.40E-31	8.10E-24
MoSe2	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Mo3Se4	3.10E-69	2.50E-58	1.70E-71	5.30E-60
NdSe	1.20E-11	3.10E-09	0.00E+00	3.70E-09
Nd2Se3	3.10E-30	7.00E-23	0.00E+00	4.50E-23
RuSe2	7.40E-34	4.60E-31	4.30E-35	2.60E-32
Sb2Se3	2.00E-55	1.00E-47	1.50E-57	2.00E-49
SmSe	5.20E-09	7.80E-06	6.80E-09	1.20E-05
USe	9.90E-11	9.10E-07	4.00E-11	3.40E-07
USe1.5	2.50E-15	1.20E-10	5.10E-16	2.50E-11
Se Condensed	2.60E-06	3.90E-05	4.10E-06	6.20E-05
Se Gas Fraction	1.30E-15	1.60E-12	4.10E-17	8.60E-14
Sm(g)	3.70E-11	2.10E-05	2.30E-11	2.00E-05
SmI3(g)	1.00E-25	2.70E-18	1.70E-25	1.80E-18
SmSe(g)	1.10E-22	1.70E-15	1.50E-23	4.10E-16
SmTe(g)	7.60E-22	9.50E-15	1.10E-22	3.00E-15
Sm Gas	3.70E-11	2.10E-05	2.30E-11	2.00E-05
Sm	1.30E-06	7.60E-05	2.20E-06	1.20E-04
Sm(l)	1.30E-06	7.60E-05	2.20E-06	1.20E-04
SmI3	2.30E-23	6.20E-20	8.20E-23	5.70E-20
SmSe	5.20E-09	7.80E-06	6.80E-09	1.20E-05
Sm Condensed	2.60E-06	1.60E-04	4.40E-06	2.50E-04
Sm Gas Fraction	1.40E-05	1.20E-01	5.30E-06	7.30E-02
Sr(g)	3.30E-07	7.50E-04	4.40E-07	2.00E-03
Sr2(g)	4.20E-12	3.10E-08	1.10E-11	2.50E-07

Pd Condensed	9.20E-07	9.20E-07	2.20E-06	2.20E-06	3.40E-06	3.40E-06
Pd Gas Fraction	4.40E-16	1.30E-15	1.20E-16	2.40E-15	9.90E-19	4.50E-17
Pu(g)	6.60E-16	2.00E-15	1.80E-16	3.70E-15	2.20E-18	1.00E-16
PuBr3(g)	8.50E-43	2.70E-42	4.80E-44	1.20E-42	1.10E-46	5.90E-45
PuI3(g)	5.40E-26	1.60E-25	5.50E-26	9.60E-25	8.40E-28	3.00E-26
PuO(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
PuO2(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Pu Gas	6.60E-16	2.00E-15	1.80E-16	3.70E-15	2.20E-18	1.00E-16
Pu(l)	2.40E-04	2.40E-04	2.30E-04	2.30E-04	2.20E-04	2.20E-04
Pu	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
PuBr3	4.10E-37	4.30E-37	6.10E-38	7.70E-38	2.00E-39	2.40E-39
PuOBr	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
PuI3	2.70E-21	2.70E-21	7.40E-21	6.50E-21	1.60E-21	1.20E-21
Pu Condensed	2.40E-04	2.40E-04	2.30E-04	2.30E-04	2.20E-04	2.20E-04
Pu Gas Fraction	2.70E-12	8.30E-12	7.90E-13	1.60E-11	9.90E-15	4.50E-13
Rb(g)	2.10E-07	6.40E-07	6.00E-07	1.20E-05	3.20E-07	1.40E-05
Rb2(g)	4.20E-12	1.30E-11	6.00E-11	1.10E-09	4.40E-11	1.90E-09
RbBr(g)	2.70E-16	8.20E-16	4.40E-16	9.10E-15	1.20E-16	5.90E-15
Rb2Br2(g)	2.40E-26	7.40E-26	1.40E-25	3.00E-24	1.10E-25	5.50E-24
RbI(g)	4.30E-10	1.30E-09	1.80E-09	3.40E-08	1.10E-09	4.60E-08
Rb2I2(g)	1.80E-14	5.40E-14	7.10E-13	1.20E-11	2.10E-12	8.10E-11
RbNa(g)	1.00E-08	3.00E-08	2.60E-08	5.10E-07	8.40E-09	3.80E-07
CsRb(g)	3.50E-10	1.00E-09	5.20E-09	9.20E-08	4.20E-09	1.80E-07
Rb Gas	2.20E-07	6.70E-07	6.20E-07	1.20E-05	3.30E-07	1.50E-05
Rb	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
RbBr	2.20E-12	2.20E-12	8.90E-12	9.30E-12	1.60E-11	1.70E-11
RbI	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
RbI(l)	1.90E-06	1.90E-06	2.00E-05	1.80E-05	6.40E-05	5.80E-05
RbI3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Rb2Se	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Rb(l)	4.30E-05	4.30E-05	2.80E-04	2.70E-04	5.30E-04	5.30E-04
Rb Condensed	4.50E-05	4.40E-05	3.00E-04	2.90E-04	6.00E-04	5.80E-04
Rb Gas Fraction	5.00E-03	1.50E-02	2.10E-03	4.00E-02	5.40E-04	2.40E-02
Rh(g)	1.40E-31	4.10E-31	2.80E-32	5.70E-31	2.60E-35	1.20E-33
Rh Gas	1.40E-31	4.10E-31	2.80E-32	5.70E-31	2.60E-35	1.20E-33
Rh(l)	3.30E-09	3.30E-09	3.20E-09	3.20E-09	2.80E-09	2.80E-09
Rh	1.10E-08	1.10E-08	1.10E-08	1.10E-08	1.10E-08	1.10E-08
Rh3U	3.00E-12	3.00E-12	2.20E-12	2.30E-12	3.60E-11	3.60E-11
Rh Condensed	1.40E-08	1.40E-08	1.40E-08	1.40E-08	1.40E-08	1.40E-08
Rh Gas Fraction	9.60E-24	2.90E-23	2.00E-24	4.00E-23	1.90E-27	8.80E-26
Ru(g)	1.20E-33	3.60E-33	3.30E-34	6.60E-33	1.20E-37	5.60E-36
Ru Gas	1.20E-33	3.60E-33	3.30E-34	6.60E-33	1.20E-37	5.60E-36
Ru	1.20E-06	1.20E-06	1.90E-06	1.90E-06	2.10E-06	2.10E-06
RuSe2	1.70E-48	1.70E-48	9.10E-50	9.10E-50	8.40E-54	8.40E-54
Ru(l)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
RuTe2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ru Condensed	1.20E-06	1.20E-06	1.90E-06	1.90E-06	2.10E-06	2.10E-06
Ru Gas Fraction	9.60E-28	2.90E-27	1.80E-28	3.50E-27	5.90E-32	2.70E-30

SrBr(g)	6.90E-12	2.70E-07	9.10E-12	7.00E-07
SrBr2(g)	1.60E-16	1.00E-10	2.50E-16	3.20E-10
SrI(g)	3.10E-10	2.50E-06	6.10E-10	6.60E-06
SrI2(g)	9.30E-14	2.80E-09	3.10E-13	8.00E-09
SrSe(g)	1.60E-19	9.60E-15	3.90E-20	5.80E-15
Sr Gas	3.30E-07	7.50E-04	4.40E-07	2.00E-03
Sr	0.00E+00	0.00E+00	0.00E+00	0.00E+00
SrBr2	3.30E-11	2.20E-09	1.40E-10	1.20E-08
SrI2(l)	1.30E-08	4.00E-08	1.10E-07	1.70E-07
Sr(l)	6.40E-04	1.50E-04	2.00E-03	5.80E-04
SrTe	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Sr Condensed	6.40E-04	1.50E-04	2.00E-03	5.80E-04
Sr Gas Fraction	5.00E-04	8.30E-01	2.20E-04	7.80E-01
Tc(g)	3.70E-24	3.60E-19	3.60E-25	5.70E-20
Tc Gas	3.70E-24	3.60E-19	3.60E-25	5.70E-20
Tc	4.10E-06	4.10E-05	6.40E-06	6.40E-05
Tc(l)	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Tc Condensed	4.10E-06	4.10E-05	6.40E-06	6.40E-05
Tc Gas Fraction	8.90E-19	8.70E-15	5.60E-20	8.80E-16
Te(g)	4.00E-18	6.20E-14	3.00E-19	9.00E-15
Te2(g)	7.30E-29	2.40E-23	1.30E-30	1.20E-24
Te3(g)	1.60E-42	1.20E-35	5.10E-45	1.60E-37
Te4(g)	9.40E-57	1.50E-48	5.50E-60	5.30E-51
Te5(g)	1.60E-68	5.60E-59	1.90E-72	5.80E-62
Te6(g)	3.30E-83	2.50E-72	7.30E-88	7.20E-76
Te7(g)	1.20E-96	1.90E-84	4.60E-102	1.40E-88
TeI2(g)	1.30E-29	2.70E-24	1.60E-30	2.70E-25
TeI4(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00
EuTe(g)	2.40E-18	2.30E-13	4.70E-19	8.70E-14
LaTe(g)	7.10E-24	1.50E-17	7.10E-25	3.50E-18
NdTe(g)	5.60E-23	1.20E-16	6.40E-24	3.20E-17
SbTe(g)	2.20E-22	7.00E-16	2.50E-23	1.90E-16
SeTe(g)	1.00E-30	3.90E-25	1.30E-32	1.30E-26
SmTe(g)	7.60E-22	9.50E-15	1.10E-22	3.00E-15
UTe(g)	2.80E-25	2.10E-17	1.00E-26	1.30E-18
UTe2(g)	1.30E-35	2.20E-26	1.50E-37	6.00E-28
YTe(g)	6.70E-26	1.00E-18	3.60E-27	1.10E-19
ZrTe2(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Te Gas	4.00E-18	6.20E-14	3.00E-19	9.00E-15
BaTe	0.00E+00	0.00E+00	0.00E+00	0.00E+00
CeTe	5.40E-10	1.10E-04	5.00E-10	1.20E-04
Cs2Te	1.10E-07	2.90E-09	2.90E-07	8.80E-09
EuTe	2.10E-05	2.10E-04	3.40E-05	4.00E-04
LaTe	1.50E-10	3.20E-08	1.30E-10	4.10E-08
La2Te3	5.80E-27	8.20E-20	1.70E-27	9.00E-20
MoTe2	0.00E+00	0.00E+00	0.00E+00	0.00E+00
NaTe(l)	0.00E+00	0.00E+00	0.00E+00	0.00E+00
NaTe3	0.00E+00	0.00E+00	0.00E+00	0.00E+00
NaTe3(l)	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Na2Te	0.00E+00	0.00E+00	0.00E+00	0.00E+00
NdTe	1.60E-10	3.40E-08	1.50E-10	4.80E-08

Sb(g)	1.20E-16	3.60E-16	8.20E-17	1.70E-15	6.80E-19	3.10E-17
Sb2(g)	2.70E-20	8.20E-20	3.30E-20	6.80E-19	1.00E-22	4.50E-21
Sb3(g)	1.90E-27	5.80E-27	3.70E-27	7.60E-26	1.50E-30	6.60E-29
Sb4(g)	2.90E-31	8.90E-31	1.10E-30	2.30E-29	2.70E-34	1.20E-32
SbBr3(g)	1.20E-65	3.80E-65	9.30E-67	2.40E-65	1.60E-71	8.70E-70
SbI3(g)	1.10E-48	3.40E-48	1.50E-48	2.70E-47	1.40E-52	5.20E-51
SbO(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
SbO2(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Sb4O6(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
SbSe(g)	1.30E-35	3.90E-35	1.70E-36	3.30E-35	1.10E-40	5.00E-39
SbTe(g)	1.80E-32	5.30E-32	1.10E-33	2.20E-32	1.20E-37	5.50E-36
Sb Gas	1.20E-16	3.60E-16	8.20E-17	1.70E-15	6.80E-19	3.10E-17
Sb	1.60E-07	1.60E-07	3.20E-07	3.20E-07	6.80E-08	6.70E-08
SbBr3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
SbI3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.40E-53	1.10E-53
Sb2Se3	8.70E-80	8.80E-80	1.60E-81	1.70E-81	1.00E-89	1.00E-89
Sb(l)	1.50E-07	1.50E-07	3.20E-07	3.20E-07	6.70E-08	6.70E-08
Sb2Te3	1.90E-71	1.90E-71	3.20E-74	3.30E-74	2.10E-82	2.10E-82
USb2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.50E-07	3.50E-07
U3Sb4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.60E-09	8.70E-09
Sb Condensed	3.10E-07	3.10E-07	6.40E-07	6.40E-07	8.80E-07	8.80E-07
Sb Gas Fraction	3.80E-10	1.20E-09	1.30E-10	2.60E-09	7.80E-13	3.50E-11
Se(g)	7.80E-33	2.40E-32	5.60E-34	1.10E-32	9.30E-38	4.20E-36
Se2(g)	1.70E-51	5.00E-51	2.30E-53	4.50E-52	3.80E-59	1.70E-57
Se3(g)	2.20E-76	6.60E-76	4.70E-79	9.40E-78	1.80E-87	8.30E-86
Se4(g)	6.50E-100	2.00E-99	2.30E-103	4.70E-102	2.90E-114	1.30E-112
SeBr2(g)	7.20E-68	2.20E-67	1.10E-69	2.60E-68	1.60E-75	8.20E-74
Se2Br2(g)	1.00E-93	3.20E-93	2.40E-96	5.60E-95	6.60E-105	3.40E-103
SeTe(g)	4.30E-48	1.30E-47	2.80E-50	5.50E-49	7.40E-56	3.30E-54
EuSe(g)	1.40E-29	4.20E-29	7.30E-30	1.50E-28	1.30E-32	6.00E-31
LaSe(g)	8.60E-36	2.60E-35	1.00E-36	2.00E-35	3.70E-40	1.70E-38
NdSe(g)	1.50E-35	4.50E-35	3.90E-36	7.80E-35	2.30E-39	1.10E-37
SbSe(g)	1.30E-35	3.90E-35	1.70E-36	3.30E-35	1.10E-40	5.00E-39
SmSe(g)	1.80E-32	5.40E-32	3.30E-33	6.60E-32	3.50E-36	1.60E-34
SrSe(g)	9.00E-30	2.70E-29	6.90E-30	1.40E-28	1.40E-32	6.40E-31
USE(g)	1.50E-40	4.50E-40	6.70E-42	1.40E-40	2.10E-46	9.60E-45
USE2(g)	5.70E-57	1.70E-56	5.50E-59	1.10E-57	3.90E-65	1.80E-63
YSe(g)	2.00E-37	6.10E-37	2.40E-38	4.80E-37	6.80E-42	3.10E-40
Se Gas	7.80E-33	2.40E-32	5.60E-34	1.10E-32	9.30E-38	4.20E-36
EuSe	1.20E-07	1.20E-07	3.00E-07	3.00E-07	4.80E-07	4.80E-07
LaSe	1.40E-14	1.40E-14	7.80E-15	7.80E-15	2.50E-15	2.50E-15
La2Se3	3.60E-41	3.60E-41	2.00E-42	2.00E-42	7.50E-45	7.60E-45
La3Se4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MoSe2	2.40E-50	2.40E-50	8.50E-52	8.50E-52	5.90E-56	5.90E-56
Mo3Se4	2.50E-104	2.50E-104	2.20E-107	2.30E-107	1.30E-115	1.30E-115
Na2Se	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Na2Se2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
NdSe	1.10E-14	1.10E-14	1.30E-14	1.30E-14	6.70E-15	6.70E-15
Nd2Se3	1.10E-40	1.10E-40	3.00E-41	3.00E-41	3.00E-43	3.00E-43
RuSe2	1.70E-48	1.70E-48	9.10E-50	9.10E-50	8.40E-54	8.40E-54
Sb2Se3	8.70E-80	8.80E-80	1.60E-81	1.70E-81	1.00E-89	1.00E-89
Se(l)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.90E-28	5.90E-28

Nd2Te3	2.30E-26	3.30E-19	8.10E-27	4.30E-19
PdTe	0.00E+00	0.00E+00	0.00E+00	0.00E+00
PdTe2	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Sb2Te3	8.30E-48	2.60E-40	9.90E-50	1.20E-41
ZrTe1.843	7.00E-21	2.00E-17	1.50E-21	8.80E-18
ZrTe2	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Zr5Te4	3.10E-52	2.60E-37	6.50E-53	4.90E-37
Te Condensed	2.10E-05	3.20E-04	3.40E-05	5.10E-04
Te Gas Fraction	1.90E-13	1.90E-10	8.70E-15	1.80E-11
U(g)	1.70E-17	5.80E-11	1.90E-18	7.60E-12
UBr(g)	4.90E-22	2.90E-14	6.00E-23	4.10E-15
UBr2(g)	5.00E-27	5.10E-18	7.00E-28	8.00E-19
UBr3(g)	7.20E-32	1.20E-21	1.20E-32	2.40E-22
UBr4(g)	1.80E-39	5.20E-28	2.70E-40	8.60E-29
UBr5(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00
UI(g)	1.10E-21	1.40E-14	1.80E-22	1.70E-15
UI2(g)	1.40E-24	6.50E-17	4.00E-25	9.10E-18
UI3(g)	1.10E-28	1.80E-20	5.10E-29	2.70E-21
UI4(g)	1.80E-33	1.00E-24	9.50E-34	1.20E-25
USE(g)	6.00E-27	5.30E-19	1.80E-28	2.40E-20
USE2(g)	5.40E-38	1.20E-28	4.20E-40	1.80E-30
UTE(g)	2.80E-25	2.10E-17	1.00E-26	1.30E-18
UTE2(g)	1.30E-35	2.20E-26	1.50E-37	6.00E-28
U Gas	1.70E-17	5.80E-11	1.90E-18	7.60E-12
U	8.50E-04	0.00E+00	8.20E-04	0.00E+00
U(l)	2.40E-05	8.70E-03	2.20E-05	5.80E-03
UBr3	3.90E-27	6.80E-21	1.80E-27	2.20E-21
UBr4	0.00E+00	0.00E+00	0.00E+00	0.00E+00
UI3	0.00E+00	0.00E+00	0.00E+00	0.00E+00
USE	9.90E-11	9.10E-07	4.00E-11	3.40E-07
USE1.5	2.50E-15	1.20E-10	5.10E-16	2.50E-11
Rh3U	0.00E+00	0.00E+00	0.00E+00	0.00E+00
URu3	5.50E-11	4.60E-05	3.60E-10	7.50E-05
USb2	0.00E+00	0.00E+00	0.00E+00	0.00E+00
U3Sb4	0.00E+00	0.00E+00	0.00E+00	0.00E+00
U Condensed	8.70E-04	8.70E-03	8.40E-04	5.90E-03
U Gas Fraction	1.90E-14	6.70E-09	2.20E-15	1.30E-09
Y(g)	4.60E-18	3.20E-12	7.60E-19	7.20E-13
YI3(g)	2.80E-26	8.90E-19	2.60E-26	3.20E-19
YSe(g)	2.40E-26	4.20E-19	1.20E-27	3.80E-20
YTe(g)	6.70E-26	1.00E-18	3.60E-27	1.10E-19
Y Gas	4.60E-18	3.20E-12	7.60E-19	7.20E-13
Y	1.00E-07	7.20E-06	1.10E-07	6.30E-06
Y(l)	8.90E-08	6.20E-06	8.60E-08	5.20E-06
YI3	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Y Condensed	1.90E-07	1.30E-05	1.90E-07	1.10E-05
Y Gas Fraction	2.40E-11	2.40E-07	4.00E-12	6.20E-08
Zr(g)	1.00E-21	1.00E-16	1.30E-22	2.10E-17
Zr2(g)	2.10E-34	2.90E-27	1.50E-35	4.00E-28
ZrBr(g)	7.90E-26	1.30E-19	1.20E-26	3.20E-20

SmSe	8.10E-10	8.10E-10	7.30E-10	7.30E-10	8.30E-10	8.30E-10
Sm2Se3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
SrSe	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
USE	7.50E-14	7.50E-14	1.90E-14	1.90E-14	1.60E-15	1.60E-15
USE1.5	3.40E-21	3.40E-21	3.80E-22	3.80E-22	5.00E-24	5.00E-24
Se Condensed	1.20E-07	1.20E-07	3.00E-07	3.00E-07	4.80E-07	4.80E-07
Se Gas Fraction	6.40E-26	1.90E-25	1.80E-27	3.60E-26	1.90E-31	8.70E-30
Sm(g)	2.10E-14	6.30E-14	2.00E-14	4.10E-13	2.20E-15	9.80E-14
SmI3(g)	1.00E-30	3.10E-30	3.10E-30	5.40E-29	1.10E-31	4.10E-30
SmO(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
SmSe(g)	1.80E-32	5.40E-32	3.30E-33	6.60E-32	3.50E-36	1.60E-34
SmTe(g)	1.50E-31	4.60E-31	1.30E-32	2.50E-31	1.30E-35	5.80E-34
Sm Gas	2.10E-14	6.30E-14	2.00E-14	4.10E-13	2.20E-15	9.80E-14
Sm(l)	2.70E-07	2.70E-07	7.40E-07	7.40E-07	1.10E-06	1.10E-06
Sm	3.60E-07	3.60E-07	9.90E-07	9.90E-07	1.70E-06	1.70E-06
SmBr3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
SmI3	2.60E-26	2.60E-26	2.20E-25	1.90E-25	1.40E-25	1.10E-25
Sm2O3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
SmSe	8.10E-10	8.10E-10	7.30E-10	7.30E-10	8.30E-10	8.30E-10
Sm2Se3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
SmTe	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Sm2Te3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Sm Condensed	6.40E-07	6.40E-07	1.70E-06	1.70E-06	2.90E-06	2.90E-06
Sm Gas Fraction	3.30E-08	9.90E-08	1.20E-08	2.30E-07	7.50E-10	3.40E-08
Sr(g)	3.90E-10	1.20E-09	1.70E-09	3.40E-08	5.70E-10	2.60E-08
Sr2(g)	6.80E-18	2.10E-17	2.20E-16	4.40E-15	5.10E-17	2.30E-15
SrBr(g)	2.10E-19	6.40E-19	5.00E-19	1.10E-17	7.30E-20	3.50E-18
SrBr2(g)	1.30E-27	3.90E-27	1.90E-27	4.40E-26	2.40E-28	1.20E-26
SrCoO2(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
SrI(g)	1.90E-13	5.60E-13	1.20E-12	2.30E-11	3.40E-13	1.40E-11
SrI2(g)	1.60E-16	4.90E-16	1.60E-15	3.00E-14	6.60E-16	2.60E-14
SrO(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
SrSe(g)	9.00E-30	2.70E-29	6.90E-30	1.40E-28	1.40E-32	6.40E-31
Sr Gas	3.90E-10	1.20E-09	1.70E-09	3.40E-08	5.70E-10	2.60E-08
Sr	3.60E-05	3.60E-05	4.00E-04	4.00E-04	1.20E-03	1.20E-03
SrBr2	1.90E-19	1.90E-19	7.90E-19	9.30E-19	2.00E-18	2.30E-18
SrI2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
SrI2(l)	3.40E-09	3.40E-09	9.40E-08	8.60E-08	4.70E-07	4.00E-07
Sr Condensed	3.60E-05	3.60E-05	4.00E-04	4.00E-04	1.20E-03	1.20E-03
Sr Gas Fraction	1.10E-05	3.30E-05	4.20E-06	8.40E-05	4.60E-07	2.10E-05
Tc(g)	9.70E-36	3.00E-35	4.20E-36	8.40E-35	1.50E-39	6.90E-38
TcO(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Tc2O7(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Tc Gas	9.70E-36	3.00E-35	4.20E-36	8.40E-35	1.50E-39	6.90E-38
Tc	1.70E-06	1.70E-06	4.10E-06	4.10E-06	6.50E-06	6.50E-06
Tc Condensed	1.70E-06	1.70E-06	4.10E-06	4.10E-06	6.50E-06	6.50E-06
Tc Gas Fraction	5.80E-30	1.70E-29	1.00E-30	2.00E-29	2.40E-34	1.10E-32
Te(g)	2.50E-28	7.70E-28	9.00E-30	1.80E-28	3.50E-33	1.60E-31
Te2(g)	2.50E-45	7.60E-45	7.70E-48	1.50E-46	3.40E-53	1.60E-51

ZrBr2(g)	2.80E-30	7.80E-23	5.20E-31	2.30E-23
ZrBr3(g)	3.10E-32	1.50E-23	1.00E-32	7.30E-24
ZrBr4(g)	3.40E-41	2.70E-31	9.20E-42	1.10E-31
ZrI(g)	1.20E-25	4.10E-20	2.20E-26	8.20E-21
ZrI2(g)	7.70E-28	9.70E-22	2.90E-28	2.50E-22
ZrI3(g)	2.50E-28	1.10E-21	2.40E-28	4.90E-22
ZrI4(g)	3.10E-36	5.00E-29	3.50E-36	1.70E-29
ZrTe2(g)	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Zr Gas	1.00E-21	1.00E-16	1.30E-22	2.10E-17
Zr	1.30E-05	1.30E-04	2.10E-05	2.10E-04
ZrBr2	2.30E-24	6.50E-21	1.60E-24	4.30E-21
ZrBr3	5.90E-33	2.90E-28	3.10E-33	1.40E-28
ZrI2	1.50E-20	1.90E-18	2.10E-20	1.20E-18
ZrI3	1.20E-28	5.50E-26	1.80E-28	2.30E-26
ZrTe1.843	7.00E-21	2.00E-17	1.50E-21	8.80E-18
ZrTe2	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Zr5Te4	3.10E-52	2.60E-37	6.50E-53	4.90E-37
Zr Condensed	1.30E-05	1.30E-04	2.10E-05	2.10E-04
Zr Gas Fraction	7.80E-17	7.60E-13	6.30E-18	9.90E-14

Te3(g)	1.10E-66	3.30E-66	2.60E-70	5.20E-69	4.90E-78	2.20E-76
Te4(g)	2.50E-88	7.70E-88	4.80E-93	9.60E-92	4.80E-103	2.20E-101
Te5(g)	2.80E-107	8.40E-107	4.20E-113	8.50E-112	2.60E-125	1.20E-123
Te6(g)	3.10E-129	9.30E-129	3.80E-136	7.50E-135	1.40E-150	6.20E-149
Te7(g)	2.50E-150	7.50E-150	2.30E-158	4.70E-157	3.90E-175	1.80E-173
Tel2(g)	9.40E-42	2.80E-41	6.50E-43	1.20E-41	7.30E-47	2.80E-45
Tel4(g)	3.00E-83	9.10E-83	2.00E-84	3.30E-83	1.90E-91	6.40E-90
EuTe(g)	4.60E-28	1.40E-27	1.10E-28	2.20E-27	2.20E-31	1.00E-29
LaTe(g)	1.20E-35	3.70E-35	6.30E-37	1.30E-35	1.90E-40	8.50E-39
NdTe(g)	1.60E-34	4.80E-34	1.80E-35	3.70E-34	1.10E-38	4.90E-37
SbTe(g)	1.80E-32	5.30E-32	1.10E-33	2.20E-32	1.20E-37	5.50E-36
SeTe(g)	4.30E-48	1.30E-47	2.80E-50	5.50E-49	7.40E-56	3.30E-54
SmTe(g)	1.50E-31	4.60E-31	1.30E-32	2.50E-31	1.30E-35	5.80E-34
UTe(g)	2.80E-38	8.40E-38	5.90E-40	1.20E-38	2.50E-44	1.10E-42
UTe2(g)	7.50E-54	2.30E-53	1.50E-56	3.00E-55	1.40E-62	6.40E-61
YTe(g)	4.80E-37	1.50E-36	2.50E-38	5.10E-37	6.10E-42	2.80E-40
ZrTe2(g)	8.00E-37	2.40E-36	9.10E-39	1.80E-37	1.30E-41	6.10E-40
Te Gas	2.50E-28	7.70E-28	9.00E-30	1.80E-28	3.50E-33	1.60E-31
Te	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
TeBr4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
BaTeO3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
BaTe	1.10E-12	1.10E-12	6.20E-13	6.20E-13	3.40E-13	3.40E-13
CeTe	2.50E-12	2.50E-12	6.40E-13	6.40E-13	1.80E-13	1.80E-13
Ce2Te3	0.00E+00	0.00E+00	2.40E-40	0.00E+00	0.00E+00	0.00E+00
Cs2Te	3.30E-10	3.20E-10	1.60E-09	1.40E-09	2.30E-09	2.10E-09
EuTe	3.30E-07	3.30E-07	3.50E-07	3.50E-07	3.60E-07	3.60E-07
LaTe	7.80E-14	7.80E-14	1.80E-14	1.80E-14	4.10E-15	4.10E-15
La2Te3	4.70E-37	4.70E-37	2.20E-39	2.30E-39	7.10E-42	7.10E-42
MoTe2	6.20E-46	6.20E-46	4.50E-48	4.50E-48	3.30E-52	3.30E-52
Mo3Te4	6.50E-97	6.50E-97	2.30E-101	2.40E-101	1.50E-109	1.60E-109
NaTe	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
NaTe(l)	4.00E-27	4.00E-27	3.80E-28	3.70E-28	1.70E-30	1.70E-30
NaTe3	1.20E-59	1.20E-59	8.30E-63	8.30E-63	5.00E-69	5.00E-69
NaTe3(l)	9.80E-73	9.80E-73	5.70E-76	5.70E-76	7.40E-83	7.40E-83
Na2Te	8.10E-24	8.10E-24	8.20E-25	8.10E-25	7.80E-27	7.80E-27
Na2Te(l)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Na2Te2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
NdTe	6.10E-14	6.10E-14	3.20E-14	3.20E-14	1.10E-14	1.10E-14
Nd2Te3	1.50E-36	1.50E-36	3.50E-38	3.50E-38	3.00E-40	3.00E-40
NpTe	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
PdTe	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.60E-28	4.60E-28
PdTe2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.40E-51	4.40E-51
PuTe	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
PuTe1.5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
RhTe	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
RhTe2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
RuTe2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Sb2Te3	1.90E-71	1.90E-71	3.20E-74	3.30E-74	2.10E-82	2.10E-82
ZrTe1.843	3.60E-30	3.60E-30	1.20E-31	1.20E-31	3.70E-34	3.70E-34
ZrTe2	2.60E-25	2.60E-25	7.30E-27	7.30E-27	6.60E-29	6.60E-29
ZrTe3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Zr5Te4	1.10E-70	1.10E-70	3.90E-73	4.10E-73	3.60E-77	3.70E-77
Te Condensed	3.30E-07	3.30E-07	3.50E-07	3.50E-07	3.70E-07	3.70E-07

<i>Te Gas Fraction</i>	7.70E-22	2.30E-21	2.60E-23	5.10E-22	9.60E-27	4.30E-25
U(g)	7.90E-26	2.40E-25	1.70E-26	3.40E-25	2.20E-29	1.00E-27
UBr(g)	2.00E-34	6.00E-34	2.50E-35	5.30E-34	2.00E-38	9.70E-37
UBr2(g)	2.40E-43	7.30E-43	1.80E-44	4.10E-43	9.40E-48	4.80E-46
UBr3(g)	1.50E-51	4.60E-51	6.80E-53	1.70E-51	3.70E-56	2.00E-54
UBr4(g)	2.80E-64	8.70E-64	7.00E-66	1.90E-64	1.20E-69	6.90E-68
UBr5(g)	2.70E-87	8.60E-87	2.80E-89	8.30E-88	1.70E-94	1.10E-92
UI(g)	1.90E-30	5.70E-30	5.80E-31	1.10E-29	5.90E-34	2.50E-32
UI2(g)	9.30E-33	2.80E-32	4.60E-33	8.50E-32	6.90E-36	2.70E-34
UI3(g)	1.70E-36	5.10E-36	1.30E-36	2.30E-35	2.70E-39	9.70E-38
UI4(g)	1.30E-42	4.00E-42	1.40E-42	2.40E-41	1.40E-45	4.70E-44
USe(g)	1.50E-40	4.50E-40	6.70E-42	1.40E-40	2.10E-46	9.60E-45
USe2(g)	5.70E-57	1.70E-56	5.50E-59	1.10E-57	3.90E-65	1.80E-63
UTe(g)	2.80E-38	8.40E-38	5.90E-40	1.20E-38	2.50E-44	1.10E-42
UTe2(g)	7.50E-54	2.30E-53	1.50E-56	3.00E-55	1.40E-62	6.40E-61
<i>U Gas</i>	7.90E-26	2.40E-25	1.70E-26	3.40E-25	2.20E-29	1.00E-27
U(l)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
U	9.10E-04	9.10E-04	8.70E-04	8.70E-04	8.40E-04	8.40E-04
UBr3	4.00E-44	4.10E-44	5.30E-45	6.60E-45	7.70E-47	9.30E-47
UBr4	4.30E-63	4.50E-63	2.50E-64	3.40E-64	1.50E-67	1.90E-67
UBr5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.60E-94	9.00E-94
UI3	4.60E-29	4.60E-29	1.10E-28	9.40E-29	5.50E-30	4.40E-30
USe	7.50E-14	7.50E-14	1.90E-14	1.90E-14	1.60E-15	1.60E-15
USe1.5	3.40E-21	3.40E-21	3.80E-22	3.80E-22	5.00E-24	5.00E-24
Rh3U	3.00E-12	3.00E-12	2.20E-12	2.30E-12	3.60E-11	3.60E-11
UPd3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
URu3	7.40E-10	7.40E-10	1.80E-09	1.80E-09	2.60E-08	2.60E-08
USb	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
USb2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.50E-07	3.50E-07
U3Sb4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.60E-09	8.70E-09
UTe	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
<i>U Condensed</i>	9.10E-04	9.10E-04	8.70E-04	8.70E-04	8.40E-04	8.40E-04
<i>U Gas Fraction</i>	8.70E-23	2.60E-22	1.90E-23	3.80E-22	2.60E-26	1.20E-24
Y(g)	1.70E-24	5.00E-24	8.70E-25	1.70E-23	6.70E-27	3.00E-25
YI3(g)	1.10E-30	3.20E-30	2.40E-30	4.20E-29	7.80E-32	2.80E-30
YSe(g)	2.00E-37	6.10E-37	2.40E-38	4.80E-37	6.80E-42	3.10E-40
YTe(g)	4.80E-37	1.50E-36	2.50E-38	5.10E-37	6.10E-42	2.80E-40
<i>Y Gas</i>	1.70E-24	5.00E-24	8.70E-25	1.70E-23	6.70E-27	3.00E-25
Y(l)	8.00E-08	8.00E-08	1.60E-07	1.60E-07	2.30E-07	2.30E-07
Y	1.60E-07	1.60E-07	3.30E-07	3.30E-07	5.50E-07	5.50E-07
YI3	5.70E-26	5.70E-26	3.60E-25	3.10E-25	1.90E-25	1.50E-25
<i>Y Condensed</i>	2.40E-07	2.40E-07	5.00E-07	5.00E-07	7.80E-07	7.80E-07
<i>Y Gas Fraction</i>	6.80E-18	2.10E-17	1.80E-18	3.50E-17	8.60E-21	3.90E-19
Zr(g)	1.30E-32	3.90E-32	5.60E-33	1.10E-31	4.00E-36	1.80E-34
Zr2(g)	5.30E-51	1.60E-50	2.80E-51	5.60E-50	9.20E-56	4.20E-54
ZrBr(g)	2.70E-40	8.30E-40	7.30E-41	1.60E-39	4.50E-44	2.20E-42
ZrBr2(g)	2.30E-48	7.20E-48	3.90E-49	9.00E-48	2.00E-52	1.00E-50
ZrBr3(g)	3.80E-52	1.20E-51	4.50E-53	1.10E-51	6.50E-56	3.60E-54
ZrBr4(g)	1.90E-66	6.10E-66	1.20E-67	3.30E-66	4.60E-71	2.70E-69
ZrI(g)	8.30E-37	2.50E-36	5.40E-37	1.00E-35	3.40E-40	1.40E-38

ZrI ₂ (g)	8.50E-38	2.60E-37	9.40E-38	1.70E-36	1.40E-40	5.30E-39
ZrI ₃ (g)	6.20E-36	1.90E-35	1.30E-35	2.30E-34	9.20E-38	3.40E-36
ZrI ₄ (g)	3.80E-45	1.20E-44	1.10E-44	1.80E-43	3.40E-47	1.10E-45
ZrTe ₂ (g)	8.00E-37	2.40E-36	9.10E-39	1.80E-37	1.30E-41	6.10E-40
Zr Gas	1.30E-32	3.90E-32	5.60E-33	1.10E-31	4.10E-36	1.90E-34
Zr(l)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Zr	1.50E-06	1.50E-06	3.50E-06	3.50E-06	4.90E-06	4.90E-06
ZrBr ₂	4.40E-38	4.50E-38	2.40E-38	2.80E-38	8.40E-40	9.50E-40
ZrBr ₃	1.30E-52	1.40E-52	3.60E-53	4.50E-53	2.40E-55	2.90E-55
ZrBr ₄	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ZrI	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ZrI ₂	5.20E-26	5.20E-26	2.00E-25	1.80E-25	2.00E-26	1.80E-26
ZrI ₃	3.70E-36	3.70E-36	1.70E-35	1.50E-35	5.20E-37	4.20E-37
ZrTe _{1.843}	3.60E-30	3.60E-30	1.20E-31	1.20E-31	3.70E-34	3.70E-34
ZrTe ₂	2.60E-25	2.60E-25	7.30E-27	7.30E-27	6.60E-29	6.60E-29
ZrTe ₃	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Zr ₅ Te ₄	1.10E-70	1.10E-70	3.90E-73	4.10E-73	3.60E-77	3.70E-77
Zr Condensed	1.50E-06	1.50E-06	3.50E-06	3.50E-06	4.90E-06	4.90E-06
Zr Gas Fraction	8.40E-27	2.60E-26	1.60E-27	3.30E-26	8.40E-31	3.80E-29

A.3 Release to Cover Gas

Figure A - 11 through Figure A - 14 present the radionuclide releases to the cover gas for both the PLOF+ ad UTOP+ transients. This includes results for both bubble sensitivity cases (“all in the bubble” and “10% in the bubble”). The plots include releases to the cover gas from bubble transport and from vaporization from the sodium pool.

Figure A - 11: PLOF+: Release to Cover Gas ("All" Case)

Figure A - 12: PLOF+: Release to Cover Gas ("10%" Case)

Figure A - 13: UTOP+: Release to Cover Gas ("ALL" Case)

Figure A - 14: UTOP+: Release to Cover Gas ("10%" Case)

A.4 Cover Gas Region and Containment Analysis

CONTAIN-LMR Issues

In the initial project plan, SNL was to use a developmental version of CONTAIN-LMR for the analysis of radionuclide behavior in the cover gas region and containment. However, several issues were encountered with the implementation of CONTAIN-LMR, which resulted in the use of the SRT code as a surrogate. This section begins with a brief overview of the CONTAIN-LMR model, followed by a discussion of the issues encountered.

Figure A - 15 shows the CONTAIN-LMR nodalization model for the reference reactor. It is comprised of 3 primary regions:

1. The first region comprises everything inside the reactor vessel. The vessel is composed of cell 2 and includes the sodium pool and cover gas region.
2. The second region comprises the containment volume. The containment nodalization from ref [1] was utilized for the current analysis. Cell 1 is located directly above the reactor vessel and cells 3 - 6 are located on the periphery of containment.
3. The third region comprises the environment. The environment is composed of cell 7.

Relevant parameters, such as pool temperatures and initial cover gas region conditions (temperatures and pressures) were specified by the results of the SAS4A/SASSYS-1 simulations, described in Section 2.2.

Figure A - 15: CONTAIN-LMR Nodalization

Five major issues were encountered during the implementation of the CONTAIN-LMR model. First, the developmental version of CONTAIN-LMR was unable to model the noble gas radionuclides as a gas, rather than an aerosol. This resulted in unrealistic removal of noble gases due to deposition. The release of noble gases is an important factor in both the PLOF+ and UTOP+ transients, as there is no retention of the noble gases within the sodium pool. This issue was rectified during the late stages of the project through changes to the CONTAIN-LMR source code.

The second issue relates to a restriction in aerosol chemical classes. The developmental version of CONTAIN-LMR only allows eight aerosol chemical classes, including one class for the noble gases and one class for sodium aerosols. Therefore, only six radionuclide classes are available for the modeling of all other radionuclide elements, if sodium aerosols and noble gases are included. For comparison, in MELCOR, it is typical to use 12 radionuclide classes (including the noble gases). Therefore, radionuclide

classes had to be combined in CONTAIN-LMR. This factor, coupled with the incorrect treatment of noble gases, made it difficult to properly evaluate the transport of radionuclides.

Third, there were difficulties encountered when attempting to institute pressure- and temperature-dependent leakage pathways from the cover gas region to the containment and from the containment to the environment. This issue resulted in the use of constant leakage rate pathways, which caused non-physical pressures in the cover gas region (pressures would reach levels below atmospheric due to the forced leakage rate to the containment), and which were no more mechanistic than the assumptions used in the SRT code.

The treatment of decay power and heat structures in CONTAIN-LMR also presented issues. If decay power is specified in the CONTAIN-LMR input, it is only maintained in the cell in which it is specified, and will not be transferred to the atmosphere or heat structure. Therefore, to model reactor vessel and containment heat-up, CONTAIN-LMR volumetric heat inputs were used in place of decay power. Using the reactor temperature plots provided by SAS4A/SASSYS-1, volumetric heat inputs were iterated upon until the pool temperatures in CONTAIN-LMR matched those from SAS4A/SASSYS-1 (pool temperatures in the UTOP+ transient are near nominal, and did not require iteration). The temperature of the cover gas region was then determined based on heat transfer from the sodium pool, and heat loss to the containment. Additionally, it is possible to model heat structures to transfer heat from the containment to the environment. However, due to the lack of a detailed reactor design, determining proper heat transfer coefficients was difficult, and initial modeling attempts using assumed values resulted in unrealistic temperatures within the containment. This factor, coupled with the incorrect treatment of cover gas region pressure, resulted in distorted aerosol behavior.

Lastly, significant code stability issues were encountered with the developmental version of CONTAIN-LMR. Resolving these issues required frequent intervention by CONTAIN-LMR/MELCOR code developers and changes to the CONTAIN-LMR source code. Utilizing CONTAIN-LMR in such a state is not a feasible pathway for an SFR industry vendor.

SRT Code Aerosol Removal Rates

As described in Section 2.7.1, the SRT code uses an exponential decay function to account for the deposition (overall removal) of airborne radionuclide aerosols. A review of past experiments was performed to determine realistic aerosol removal rates in both the cover gas region and containment. The main source of data was a series of sodium aerosol experiments performed at the Hanford Engineering Development Laboratory (HEDL) in the late 1970s and early 1980s [2-5].

The HEDL tests were conducted in the Containment Systems Test Facility (CSTF), which was a simulated containment vessel with the properties provided in Table A - 4. In total six (documented) experiments were conducted to examine the behavior of sodium aerosols. Table A - 6 provides a short description of each of the six AB tests, which included both sodium pool and spray fires, with and without the addition of NaI aerosols.

Table A - 4: CSTF Properties

Property	Value
<i>Height</i>	<i>20.3m</i>
<i>Diameter</i>	<i>7.62m</i>
<i>Volume</i>	<i>852m³</i>
<i>Volume-to-Height Ratio</i>	<i>41.97</i>

Table A - 5: AB Tests Description

Test	Description
AB1	Sodium pool fire (410kg)
AB2	Sodium pool fire (472kg) with steam addition to containment
AB3	Sodium spray fire (48kg, 670 μ m MMD ¹)
AB5	Sodium spray fire (223kg, 1030 μ m MMD)
AB6	Sodium spray fire (205kg, 640 μ m MMD) with NaI aerosol addition
AB7	Sodium pool fire (6.4kg) with NaI aerosol addition

¹Mass Median Diameter

For the current analysis, the most pertinent result of the AB tests is the airborne aerosol removal rate from the containment vessel following the termination of the sodium pool or spray fire. This information provides insight into the level of aerosol removal that might be seen in the reference reactor containment, following radionuclide and sodium aerosol release from the cover gas region (aerosol removal from the cover gas region will be discussed at the end of this subsection). The aerosol concentration was recorded for all six AB experiments, with separate measurements of NaOH and NaI aerosol concentration for tests AB6 and AB7. Based on this information, average aerosol removal rates were calculated, as part of the current project, provided in Table A - 6. The aerosol removal rates were remarkably consistent across all tests, except for NaI aerosol removal in AB6, but this result was likely influenced by the termination of NaI aerosol injection before the completion of the sodium spray fire. The aerosol removal rates are also very similar to those seen in other sodium aerosol experiments, such as the FAUNA pool fire tests, which returned average aerosol removal rates of approximately 4e-5 per second [6].

Table A - 6: HEDL AB Tests Average Aerosol Removal Rates

Test	Average Removal Rate (s⁻¹)
AB1	3.1e-5
AB2	3.8e-5
AB3	4.2e-5
AB5	4.8e-5
AB6 NaI	3.1e-4
AB6 NaOH	4.1e-5
AB7 NaI	3.9e-5
AB7 NaOH	4.6e-5

Compared to the reference reactor containment, the CSTF containment used in the AB tests had a much lower volume-to-height ratio (190.1 for the reference reactor, compared to 41.97 for the CSTF). Gravitational settling is likely the dominant aerosol removal mechanism for the cases analyzed as part of the trial MST. The higher volume-to-height ratio of the reference reactor containment should result in higher aerosol removal rates compared to similar aerosol loading in a containment with a volume-to-height ratio of the CSTF. Scoping containment calculations were performed with CONTAIN-LMR, with aerosol properties based on ref [7]. The CONTAIN-LMR calculations returned an aerosol removal rate of approximately 5.5e-5 per second in the containment volume. This value was utilized for the trial MST analysis, as it is similar to the average results seen from the AB tests, with a slight increase to account for the differences in the containment volume and height. For comparison purposes to LWR aerosol removal rates, the AP1000 containment analysis utilized aerosol deposition rates ranging from 1.37e-4 to 4.72e-4 per second, neglecting steam condensation on airborne particles [8].

For aerosol removal in the cover gas region, an additional set of CONTAIN-LMR scoping calculations were performed. The calculations resulted in an aerosol removal rate of 1.1e-4 per second, which was considerably higher than within the containment. This difference is likely a result of the significantly smaller volume and the high volume-to-height ratio.

Appendix B: Sensitivity Calculation Details

The following sections provides further details regarding the sensitivity calculation reviewed in Section 3. This begins with a review of the source term analysis tool, and is followed by complete results from the eight base cases and sensitivity analyses.

B.1 Source Term Sensitivity Analysis Tool

The source term sensitivity tool was developed to support the performance of sensitivity studies associated with the different components of source term analysis for an SFR. Development of the tool was performed by treating the various processes that reduce the source term during radionuclide transport to the environment as first order processes involving fractional removal rates that are proportional to the density of radionuclides present. Differential equations were developed associated with the mass balance for a control volume. These were then integrated over the duration of the event. For the cases involving small release rates from the cover gas region, the equations were developed for four compartments. When it was assumed that primary system integrity had been lost as the result of accident processes (or that the plant design bases do not assure the integrity of the primary system). All scenarios began with the release of radioactive material from all affected fuel elements, which was assumed to be rapid (effectively instantaneous). Transport through the sodium pool was also assumed to be instantaneous for the bypass portion of the release.

Definition of Terms

I_i = dose weighted inventory for radionuclide i
 f_{FRi} = Fuel release fraction for radionuclide i
 f_{PRi} = Sodium pool release fraction for radionuclide i
 f_B = Bypass fraction (1/DF)
 λ_p = primary system release rate (fraction per section)
 λ_c = containment system release rate (fraction per section)
 λ_{di} = decay rate for radionuclide i (fraction per section)
 λ_a = aerosol deposition rate (fraction per section)
 t_e = end time of scenario (s)
 L = fractional release rate of sodium to containment
 ST_{CGi} = Integrated source term to cover gas region for radionuclide i
 ST_{Ci} = Integrated source term to containment region for radionuclide i
 ST_{Ei} = Integrated source term to environment for region i

Four-Node Analysis

Source Term to Cover Gas Region

$$ST_{CGi} = (f_B f_{FRi} + (1 - f_B) f_{FRi} L f_{PRi} t_e) I_i$$

Source Term to Containment

$$ST_{Ci} = \frac{\lambda_p f_B f_{FRi} I_i}{\lambda_{di} + \lambda_p} \left(1 - e^{-(\lambda_{di} + \lambda_p) t_e} \right) + \frac{\lambda_p (1 - f_B) f_{FRi} L f_{PRi} I_i}{\lambda_{di} + \lambda_p} \left(t_e - \frac{(1 - e^{-(\lambda_p + \lambda_{di}) t_e})}{\lambda_{di} + \lambda_p} \right)$$

Source Term to Environment

$$\begin{aligned}
ST_{Ei} = & -\frac{\lambda_c \lambda_p f_B f_{FRI} I_i}{\lambda_c + \lambda_a - \lambda_p} \left(\frac{(e^{-(\lambda_{di} + \lambda_p)t_e} - 1)}{\lambda_{di} + \lambda_p} - \frac{(e^{-(\lambda_{di} + \lambda_a + \lambda_c)t_e} - 1)}{\lambda_{di} + \lambda_a + \lambda_c} \right) + \\
& + \frac{\lambda_c \lambda_p (1 - f_B) f_{FRI} f_{PRI} L I_i}{\lambda_p + \lambda_{di}} \left(\frac{(e^{-(\lambda_{di} + \lambda_p)t_e} - 1)}{(\lambda_{di} + \lambda_p)(\lambda_{di} + \lambda_a + \lambda_c)} - \frac{(e^{-(\lambda_{di} + \lambda_c + \lambda_a)t_e} - 1)}{(\lambda_{di} + \lambda_a + \lambda_c)(\lambda_c + \lambda_a - \lambda_p)} \right. \\
& \left. + \frac{(e^{-(\lambda_{di} + \lambda_c + \lambda_a)t_e} - 1)}{(\lambda_{di} + \lambda_a + \lambda_c)^2} + \frac{t_e}{(\lambda_{di} + \lambda_a + \lambda_c)} \right)
\end{aligned}$$

Three-Node AnalysisSource to Containment

$$ST_{Ci} = f_B f_{FRI} I_i + (1 - f_B) f_{FRI} I_i L t_e$$

Source to Environment

$$ST_{Ei} = \frac{\lambda_c f_B f_{FRI} I_i}{\lambda_c + \lambda_a + \lambda_{di}} (1 - e^{-(\lambda_c + \lambda_a + \lambda_{di})t_e}) + \frac{(1 - f_B) \lambda_c f_{FRI} f_{PRI} L I_i}{\lambda_c + \lambda_a + \lambda_{di}} \left(t_e + \frac{(e^{-(\lambda_{di} + \lambda_c + \lambda_a)t_e} - 1)}{(\lambda_{di} + \lambda_a + \lambda_c)} \right)$$

B.2 Detailed Base Cases Results

This section provides complete results of dose contributors and land contamination rankings for the eight base cases described in Section 3.3.

Figure B - 1: Case Study 1 – Dose Contributors

Figure B - 2: Case Study 1 – Land Contamination

Figure B - 3: Case Study 2 – Dose Contributors

Figure B - 4: Case Study 2 – Land Contamination

Figure B - 5: Case Study 3 – Dose Contributors

Figure B - 6: Case Study 3 – Land Contamination

Dose Contributors
Figure B - 7: Case Study 4 - Dose Contributors

Figure B - 8: Case Study 4 - Land Contamination

Figure B - 9: Case Study 5 - Dose Contributors

Figure B - 10: Case Study 5 – Land Contamination

Dose Contributors
Figure B - 11: Case Study 6 - Dose Contributors

Figure B - 12: Case Study 6 - Land Contamination

Figure B - 13: Case Study 7 – Dose Contributors

Figure B - 14: Case Study 7 - Land Contamination

Dose Contributors
Figure B - 15: Case Study 8 - Dose Contributors

Figure B - 16: Case Study 8 - Land Contamination

B.3 Detailed Sensitivity Analysis Results

This section provides detailed results regarding the sensitivity analysis described in Section 3.4. Specifically, side-by-side comparisons are provided between the base case results and the results with the modified input values regarding radionuclide transport. The results are presented in the following order:

- Sodium Pool Bypass
 - Case Study 1.1 – Page B-21
 - Case Study 2.1 – Page B-21
 - Case Study 3.1 – Page B-22
 - Case Study 4.1 – Page B-22 and B-23
- Containment Aerosol Deposition
 - Case Study 2.2 – Page B-24
 - Case Study 4.2 – Page B-24
- Actinide/Lanthanide Fuel Release Fractions
 - Case Study 2.3 – Page B-25
 - Case Study 4.3 – Page B-25

Figure B - 17: Case Study 1 - DF=3

Figure B - 18: Case Study 2 - DF=3

Figure B - 19: Case Study 1.1 - DF=30

Figure B - 20: Case Study 2.1 - DF=30

Figure B - 25: Case Study 4 - DF=10 **Figure B - 26: Case Study 4.1 - DF=1000 (Axis Change)**

Figure B - 31: Case Study 2 – Degraded Primary **Figure B - 32: Case Study 4 – Degraded Primary** **Figure B - 33: Case Study 2.3 – Degraded Primary, Ac/La RF=0.0001** **Figure B - 34: Case Study 4.3 – Degraded Primary, Ac/La RF=0.0001**

Appendix C: Thermodynamic Database

The following section provides further detail regarding the custom thermodynamic database created for HSC Chemistry 8 as part of the current effort.

C.1 Summary of Thermodynamic Modeling Approach

To determine the partitioning of key elements between gas phases (pin plenum, bubbles, cover gas) and condensed phases (liquid sodium, precipitates), thermodynamic equilibrium speciation calculations were performed using the Gibbs free energy minimization module of the HSC Chemistry 8 software package [9]. The generic components and information flow for a thermodynamic source term calculation, such as the one summarized in this report, are shown in Figure C-1.

Figure C-1: Schematic Information Flow Diagram for the HSC Chemistry Thermodynamic Calculations²

The key to model accuracy and applicability is the thermodynamic database that contains the constants (standard enthalpies and entropies) used to calculate the system's Gibb's energy and the heat capacities that are used to quantify temperature dependencies (top line, Figure C-1). To account for non-ideal mixing, Gibbs free energy excess functions must be obtained from the literature or by focused experimentation, as they are not included in the database that comes with the HSC Chemistry code. For this study, the Gibbs free energy excess functions, quantified as activity coefficients (discussed in section C.2), were derived from relevant experimental and thermodynamic studies.

² RN used as abbreviation for radionuclides.

Once the thermodynamic databases and mixing models are compiled, the user specifies the bulk composition (pin or pool radionuclide inventory), the temperature (uniform throughout system) and either the pressure or volume of the system (if pressure is specified the volume is calculated and vice versa). Similar to many other thermodynamic modeling codes, HSC Chemistry 8 works by first identifying all possible chemical species and phases that could form from a user specified bulk chemical composition and then determining the equilibrium speciation (amounts of specific compounds) of the system by minimizing the total Gibbs free energy of the system for a specified temperature and pressure (or volume). The user specified bulk composition represents the reactants in the system while the calculation results represent the assemblage of stable products for the specified bulk composition, pressure, and temperature conditions. Discussions of the model's theoretical basis, and the custom thermodynamic database compiled for this study are provided in Section C.2 below.

It is important to note that equilibrium models have inherent limitations stemming from several commonly unrealistic basic assumptions such as:

- The homogeneous mixing of all phases and species,
- The absence of chemical and thermal gradients,
- The absence of kinetic constraints on precipitation, melting, dissolution, vaporization.

However, when using the equilibrium modeling approach to calculate radionuclide release and transport, not accounting for these kinetic phenomena result in conservative predictions making the results instructive and appropriate for use in quantifying accident scenario source terms. Furthermore, with a sufficiently thorough database and experimental validation, equilibrium models offer the advantage of providing a predictive tool for assessing complex, multiphase systems that cannot be fully understood by site measurements and experimentation alone. Furthermore, equilibrium models can rapidly account for complex chemical interactions and interdependencies that may be missed in simplified experiments and accident site characterizations.

C.2 Compilation of Custom HSC Chemistry Thermodynamic Database

The thermodynamic driving force responsible for the release of fission products from the liquid sodium coolant into the cover gas is the equilibrium vapor pressure at a specified pressure, temperature, and bulk composition. The kinetics of release are influenced by the coolant fluid dynamics, liquid surface area, activation energies, and other scenario-specific factors. Since many of these kinetic influences are poorly quantified or will be unknown for a particular accident scenario the chemical model used in this study is based on the primary thermodynamic mechanism for release, which is equilibrium vaporization at a specific pressure, temperature, and liquid composition. The model is conservative with respect to kinetic factors in that we assume that the radionuclide equilibrium vapor pressures are achieved instantaneously.

Equilibrium vapor pressures are quantified in HSC Chemistry 8 using a variation of the Redlich-Kwong equation of state and a standard Gibbs free energy minimization algorithm that calls a thermodynamic database populated with species-specific standard values for enthalpy, entropy and heat capacities [9]. The Gibbs free energy minimization is achieved by a standard Lagrangian-multiplier numerical method. The thermodynamic database supplied with the commercial HSC Chemistry 8 software was compiled from open literature sources and accounts for thousands of solid, liquid, and gas species; however, some of the constants used for key fission product species (e.g., salts of iodine, bromine, tellurium, and selenium) are either missing or are estimates for which more certain values exist. These constants are easily updated using the thermodynamic database editing module in the HSC code that allows the user to compile a custom database that can be used simultaneously (in addition to) the standard HSC Chemistry database for a given calculation.

For the present study a custom database was created by replacing zero values for key constants with values obtained from the literature as well adding thermodynamic constants that quantify non-ideal mixing behavior. The constants that were compiled include standard enthalpies, entropies and heat capacity parameters. The important relationships between these constants and parameters and the Gibb's free energy are as follows:

$$\Delta G = \Delta H - T\Delta S \quad \text{C-Eq.1}$$

$$\Delta H(T) = \Delta H_f^o + \int_{298K}^T C_p dT + \sum(\Delta H_t) \quad \text{C-Eq.2}$$

$$\Delta S(T) = \Delta S_f^o + \int_{298K}^T \left(\frac{C_p}{T}\right) dT + \sum\left(\frac{\Delta H_t}{T_t}\right) \quad \text{C-Eq.3}$$

Where (G) is the Gibbs free energy, (H) is enthalpy, (S) is entropy, (C_p) is heat capacity and (T) is temperature. The symbol (o) indicates standard state (298.15 K, 1 bar), (f) stands for formation and (t) denotes phase transformation.

An example section of the custom database is shown in Table C-1. All HSC formatted databases use a variation of the empirical Kelley equation (C-Eq.4) to parameterize the temperature dependence of the thermodynamic constants [9].

$$C_p(T) = A + BT \times 10^{-3} + CT^{-2} \times 10^5 + DT^2 \times 10^{-6} \quad \text{C-Eq.4}$$

Table C-1: Example Section of the Custom HSC Chemistry 8 Thermodynamic Database Compiled for the Present Study

Species	ΔG^o (kJ/mol)	Melting T (K)	Boiling T (K)	ΔH^o (kJ/mol)	ΔS^o (J/mol K)	A*	B*	C*	D*	Reference
Na	Calculated	371	n/a	0	51.3	21.14	22.50	-0.11	11.01	Knacke, 91 [10]
Na(l)	Calculated	n/a	1156	2.60	57.86	38.13	-19.51	-0.70	10.25	Nasa, 93 [11]
Na(g)	Calculated	n/a	n/a	107.5	153.71	20.82	-0.10	-0.01	0.05	Landolt, 99 [12]
NaI	Calculated	934	n/a	-287.86	-98.50	41.97	25.19	2.32	-10 ⁻³	Barin, 93 [13]
NaI(l)	Calculated	n/a	1577	-266.51	120.75	41.97	25.19	2.32	-10 ⁻³	Glushko, 94 [14]
NaI(g)	Calculated	n/a	n/a	-90.63	248.97	37.35	0.72	-0.83	0.15	Glushko, 94 [14]
Cs	Calculated	301.60	n/a	0.0	85.23	58.57	-246.2	-1.36	546.4	Landolt, 99 [12]
Cs(l)	Calculated	n/a	944.0	2.20	92.55	49.48	-48.20	-4.55	29.45	Landolt, 99 [12]
Cs(g)	Calculated	n/a	n/a	76.50	175.59	20.82	-0.12	-0.002	0.089	Landolt, 99 [12]
CsI	Calculated	894.0	n/a	-348.1	122.2	61.10	-39.97	-1.41	54.93	Glushko, 94 [14]
CsI(l)	Calculated	n/a	1553.0	-266.51	120.75	41.96	25.19	2.322	-10 ⁻³	Glushko, 94 [14]
CsI(g)	Calculated	n/a	n/a	-152.32	275.28	37.99	-0.12	-0.52	0.53	Glushko, 94 [14]

* Heat capacity parameters, see equation C-Eq.4.

This database does not; however, include the thermodynamic excess functions needed to quantify equilibrium speciation in the complex mixtures of interest, i.e. fission products and actinides dissolved in liquid sodium. For this reason, the relevant excess functions that account for non-ideal mixing, were compiled and added to the custom thermodynamic database used for this project.

The compilation of the custom database involved using or deriving activity coefficients from relevant experimental investigations (discussed below). The activity coefficients (γ) are related to the excess Gibbs free energy of species i in a mixture (ΔG_i^{Excess}) by the following equations:

$$\Delta G_i^{Excess} = \Delta G_i^{Real} - \Delta G_i^{Ideal} \quad \text{C-Eq.5}$$

Where ΔG_i^{Real} and ΔG_i^{Ideal} refer to the partial molar Gibbs free energy for the real mixture and the thermodynamically ideal mixture respectively.

$$\Delta G_i^{Excess} = \Delta H_i^{Mixing} - T\Delta S_i^{Excess} \quad \text{C-Eq.6}$$

Where ΔH_i^{Mixing} is the partial molar heat of mixing and ΔS_i^{Excess} is the partial molar excess entropy of mixing. The activity coefficient (γ_i), which is a factor that accounts for the non-ideal chemical behavior of species i in a mixture, is related to the Gibb's excess energy by:

$$\gamma_i = \exp \left(\frac{\Delta G_i^{Excess}}{RT} \right) \quad \text{C-Eq.7}$$

The activity coefficients for particular species of interest were derived from relevant experimental studies and tabulated within the HSC Chemistry database so that they were applied in all of the modeling scenarios that were implemented for this project.

All of the experimental studies looked at for this project reported their equilibrium partitioning measurements in terms of partition coefficients (Kd_i). The relationship between the partition coefficient and the activity coefficient for a case where the fission product element i is mixed within a relatively large mass of sodium are:

$$\gamma_i = \frac{P_{Na}^o Kd_i}{P_i^o} \quad \text{C-Eq.8}$$

Where P_{Na}^o is the standard vapor pressure of pure sodium, and P_i^o is the standard vapor pressure of fission product i . The partition coefficient (Kd_i) is defined by:

$$Kd_i = \frac{[n_i/(n_i+n_{Na})]_{vap}}{x_i} = \frac{[P_i/(P_{Na}+P_i)]_{vap}}{x_i} \quad \text{C-Eq.9}$$

Where n_i is the number of moles of vapor species i , n_{Na} is the number of moles of the “solvent” liquid (in the case of interest: sodium), P is partial pressure, and x_i is the mole fraction of species i .

And therefore:

$$Kd_i = \frac{\gamma_i P_i^o}{\gamma_i x_i P_i^o + \gamma_{Na} x_{Na} P_{Na}^o} \quad \text{C-Eq.10}$$

And since, for the case of interest (low concentrations of radionuclides in a relatively large volume of sodium liquid):

$$P_i \ll P_{Na} \text{ and } x_i \ll (1-x_i)$$

$$\text{we can assume } P_{Na} = P_{Na}^o$$

Therefore:

$$Kd_i = \frac{P_i}{(P_{Na}^o x_i)} = \frac{\gamma_i P_i^o}{P_{Na}^o} \quad \text{C-Eq.11}$$

The custom database was compiled for mixtures of the key fission product elements Ba, Br, Cs, Rb, Sr, I, and Te. There are many uncertainties and unknowns in the current custom database due a lack of relevant experimental data for fission product – liquid sodium mixtures. New experimental studies are needed to fill these information gaps. The experiments that were used to derive the activity coefficients discussed

below were those of Castleman and Tang (1968) [15], Wichner et al. (1984) [16], Haga et al. (1992) [17], and Miyahara et al., (2011) [18]. The thermodynamic discussions provided by Schram et al. (1995) [19] were also used extensively in formulating the custom activity coefficient functions used in this study.

The Castleman and Tang (1968), Pollock et al. (1968), and Clough (1969) used distillation methods to quantify the partition coefficients for Cs, I, and Te from liquid Na at temperatures of 450°C to 500°C. More recent studies by Haga et al. (1992) and Miyahara et al. (2011) used a transpiration method to measure the partition coefficients of these volatile fission products over a broader temperature range 450°C – 850°C.

Haga et al. (1992) and Miyahara et al. (2011) were the primary sources used to determine the activity coefficients for Cs, I, and Te in the present study because of the relevance of their experimental temperature ranges to the accident scenarios of interest. It is worth summarizing the experimental details from these studies, as their methodology represents a promising approach to filling information gaps identified in this report (i.e. measuring activity coefficients for specific fission product species that are currently unknown).

Both the Haga et al. (1992) and Miyahara et al. (2011) sets of experiments used the same experimental set up, which consisted of a 304 stainless steel vessel filled with 50 grams of sodium and contained within an electric furnace. The experimental set up for these experiments is shown schematically in Figure C-2. Metallic cesium, crystalline NaI and CsI particles or Te powder are mixed with the sodium at the beginning of each experiment. The sodium surface area for this set up was 74cm² and the sodium depth was 12mm. Thermocouples were positioned throughout the test apparatus, both within the liquid sodium and within the cover gas. During each experiment a gas sample was taken from directly above the gas/liquid sodium interface using a (syringe type device), since the gas phase directly adjacent to the sodium interface is most likely to have achieved equilibrium with respect to the partitioning of volatile species between liquid and gas. The gas phase temperature was kept 3°C to 13°C higher than that of the liquid phase to prevent sodium mist formation. The Ar purge gas was presaturated with respect to the sodium - fission product mixture prior to flow through the experimental vessel. Aerosols were filtered out the purge gas using steel filters. Gas samples were condensed and analyzed for cesium and tellurium by either atomic absorption analyses or Inductively Coupled Plasma-Mass Spectroscopy and for iodine by ion chromatography (Haga et al., 1992, Miyahara et al., 2011).

Figure C-2: Schematic Diagram of Experimental Apparatus Used to Measure the Equilibrium Vaporization Pressures of Key Radionuclide Elements over Liquid Sodium at Constant Temperature and Pressure (Adapted from (Haga et al., 1992))

As shown in equations C-Eq.8 to C-Eq.11 the conversion between Kd_i , P_i and γ_i requires values for the vapor pressure of the pure phase, denoted as P_i^o , where i is Na, Cs or NaI. The temperature dependence of the pure phase vapor pressures of interest are shown below (from Miyahara et al., 2011).

$$\log(P_{Na}^o) = 5.47838 - \frac{5383.69}{T} - 0.27760 \log(T) \quad \text{C-Eq.12}$$

$$\log(P_{Cs}^o) = 5.57298 - \frac{3893.87}{T} - 0.51054 \log(T) \quad \text{C-Eq.13}$$

$$\log(P_{NaI}^o) = 8.81998 - \frac{9305.03}{T} - 0.90885 \log(T) \quad \text{C-Eq.14}$$

Figures C-3 – C-6 provide the comparison of the HSC Chemistry model results, obtained using the custom database, versus relevant experimental data from which the activity coefficient functions were derived. The most illustrative means to compare the thermodynamic modeling results to the experimental data is by plotting values in terms of partial pressures of equilibrium species versus temperature. This allows for the comparison of the direct output of the model to a physically measurable quantity. The relationship between the (Kd_i) value and the partial pressure of the volatile fission product (P_i) is given in C-Eq.11 above.

The plots shown below give a qualitative sense of the uncertainties involved in deriving activity coefficients from experimental data and also show the effect of underlying assumptions. The three possible underlying assumptions are:

- 1) System is a nonideal mixture (uses activity coefficient function derived in this study)
- 2) System is an ideal mixture
- 3) System is composed of non-mixing pure phases

Figure C-3: Plots of the Experimentally Determined Activity Coefficients for Cs and NaI in Liquid Sodium and the Function Derived for Use in the Present Study (red dotted line)

Figure C-3 shows relatively good agreement of the activity coefficient function used in the present study with the experimental data. All of the activity coefficient functions derived for this study are shown in Table C-2. To give further perspective on the derived activity coefficient functions, HSC Chemistry model runs were performed for Cs, I and Te in liquid sodium assuming three different conditions: (1) realistic mixing (custom database sued), (2) realistic mixing with derived activity coefficients multiplied by a factor of 2, (3) ideal mixing, and (4) only pure phases present (no mixing). The results (Figure C-4) show that the ideal mixing assumption under predicts the equilibrium vapor pressure of Cs over liquid Na, while

the pure phase assumption dramatically over predicts the partitioning of Cs into the gas phase. Using the realistic custom database provides the result most consistent with the experimental results.

Figure C-4: Results from Equilibrium Partial Pressure Experiments Showing Predictions from the HSC Chemistry Code for Different Assumptions

Figure C-5: Partial Pressure of NaI(g) over Na for the Three Different Assumptions Discussed Above

Figure C-5 indicates that for NaI in Na, the realistic mixture (custom database) assumption is in fairly good agreement with experimental data. While the ideal mixture assumption results in under prediction of NaI volatilization. Multiplying the activity coefficients by 2x is also shown as an example of the sensitivity of vapor pressure to the activity coefficient values. Figure C-6 shows the limited data set for Te in Na, it is interesting to note in this case that, the derived Te activity coefficient over predicts Te volatilization below 600°C. This discrepancy is likely due to uncertainty in the pure phase vapor pressure of Na_2Te (P_i^0 in equations C-Eq.8 - 11), which is needed to convert between activity coefficients and partial pressures.

Figure C-6: Experimental Data for Te in Liquid Sodium Showing the Activity Coefficients and Derived Function (Red Line) (Left) and the Predicted Te Partial Pressures

A complete list of the activity coefficient functions used for the present study is shown in Table C-2. The form of these equations is dictated in part by the requirement that they involve simple operations and that they be in the form of a natural logarithm.

Table C-2: Activity Coefficient Functions Used for this Study and the Literature Sourced from which they were Derived

<i>Element in Na liquid</i>	<i>Activity coefficient function $\ln \gamma_i =$</i>	<i>Source from which activity coefficient function was derived</i>
Ba	$2.113/0.008314 \cdot T$	The activity coefficient for strontium was calculated using equation C-Eq.7 from the excess Gibbs energy function determined by Schram et al., 1995 through analyses of the Ba-Sr phase diagram.
xBr	$57.3 - 0.025 \cdot T / 0.0083145 \cdot T$	The activity coefficient for bromide salts was calculated from the excess Gibbs energy (equation C-Eq.7) determined by Pitzer, 1962 [20] from a phase diagram analyses (liquidus activities) within the temperature range 747°C to 957°C.
Cs	$2.303 \cdot (240/T + 0.0585)$	Haga et al., 1992, Miyahara et al., 2011 see discussion above.
Rb	$(7.52 - 0.0000282 \cdot T) / 0.0083145 \cdot T$	The activity coefficient for bromide salts was calculated from the excess Gibbs energy (equation C-Eq.7) determined by Bale, 1982 [21].
Sr	$8.352 / 0.008314 \cdot T$	The activity coefficient for strontium was calculated using equation C-Eq.7 from the excess Gibbs energy function determined by Schram et al., 1995 through analyses of the Na-Sr phase diagram.
xI	$2.303 \cdot (3475/T - 1.486)$	Haga et al., 1992, Miyahara et al., 2011 see discussion above.
xTe	$(24.5 - 0.0239 \cdot T) / 0.0083145 \cdot T$	Haga et al., 1992, Miyahara et al., 2011 see discussion above.
xSe	Assumed to be in ideal mixture	Information gap
Lanthanides	Assumed to be in ideal mixture	Information gap
Actinides	Assumed to be in ideal mixture	Information gap

The excess functions for the other key species such as the selenide salts, and antimony, zirconium, lanthanide, and actinide compounds, are unknown for sodium mixtures and were thus treated as an ideal mixtures. The lack of thermodynamic constants for these elements is a source of uncertainty in this study and represents a significant information gap. Such gaps need to be addressed by new experimental and thermodynamic studies in order to reduce the significant uncertainties in mechanistic assessments of accident scenario radionuclide source terms.

Tables C-3 and C-4 below list all of the gas and condensed species that were considered in the HSC Chemistry thermodynamic calculations for this study. To the point made above, many of these species need further study to reduce uncertainties in the source term calculations.

Table C-3: List of All 241 Gas Species Considered in HSC Chemistry 8 Thermodynamic Equilibrium Calculations for Both the Pin → Plenum → Bubble and the Sodium Pool → Cover Gas Releases

Am(g)	EuBr2(g)	MoO(g)	PuO(g)	SeTe(g)	UI2(g)
Ba(g)	EuI3(g)	MoO2(g)	PuO2(g)	Sm(g)	UI3(g)
Ba2(g)	EuO(g)	MoO3(g)	Rb(g)	SmI3(g)	UI4(g)
BaBr(g)	Eu2O(g)	MoOBr3(g)	Rb2(g)	SmO(g)	UO(g)
BaBr2(g)	Eu2O2(g)	MoOBr4(g)	RbBr(g)	SmSe(g)	UO2(g)
BaI(g)	EuSe(g)	MoO2Br2(g)	Rb2Br2(g)	SmTe(g)	UO3(g)
BaI2(g)	EuTe(g)	Na(g)	RbI(g)	Sr(g)	U2O2(g)
BaMoO4(g)	I(g)	Na2(g)	Rb2I2(g)	Sr2(g)	U2O3(g)
BaO(g)	I2(g)	NaBr(g)	RbNa(g)	SrBr(g)	U2O4(g)
Ba2O(g)	I3(g)	Na2Br2(g)	RbO(g)	SrBr2(g)	U2O5(g)
Ba2O2(g)	IBr(g)	NaI(g)	Rb2O(g)	SrCoO2(g)	U2O6(g)
Br(g)	IO(g)	Na2I2(g)	Rb2O2(g)	SrI(g)	USe(g)
Br2(g)	IO2(g)	NaO(g)	Rh(g)	SrI2(g)	USe2(g)
BrO(g)	IO3(g)	Na2O(g)	RhO(g)	SrO(g)	UTe(g)
BrO2(g)	Kr(g)	Na2O2(g)	RhO2(g)	SrSe(g)	UTe2(g)
BrOO(g)	La(g)	Nb(g)	Ru(g)	Tc(g)	Xe(g)
BrO3(g)	La2(g)	NbBr5(g)	RuO(g)	TcO(g)	Xe2(g)
Br2O(g)	LaBr3(g)	NbBr3O(g)	RuO2(g)	Tc2O7(g)	Y(g)
BrBrO(g)	LaI3(g)	NbI2(g)	RuO3(g)	Te(g)	Y2(g)
BrOBr(g)	LaO(g)	NbI3(g)	RuO4(g)	Te2(g)	YBr2(g)
Ce(g)	LaO2(g)	NbI4(g)	Sb(g)	Te3(g)	YI2(g)
Ce2(g)	La2O(g)	NbI5(g)	Sb2(g)	Te4(g)	YI3(g)
CeBr3(g)	La2O2(g)	NbO(g)	Sb3(g)	Te5(g)	YO2(g)
CeI3(g)	LaRh(g)	NbO2(g)	Sb4(g)	Te6(g)	Y2O(g)
CeO(g)	LaSe(g)	NbOI3(g)	SbBr3(g)	Te7(g)	Y2O2(g)
CeSe(g)	LaTe(g)	Nd(g)	SbI3(g)	TeI2(g)	YSe(g)
CeTe(g)	Mo(g)	NdBr3(g)	SbO(g)	TeI4(g)	YTe(g)
Cs(g)	Mo2(g)	NdI3(g)	SbO2(g)	TeO(g)	Zr(g)
Cs2(g)	MoBr(g)	NdO(g)	Sb4O6(g)	TeO2(g)	Zr2(g)
CsBr(g)	MoBr2(g)	NdSe(g)	SbSe(g)	TeO3(g)	ZrBr(g)
Cs2Br2(g)	MoBr3(g)	NdTe(g)	SbTe(g)	Te2O2(g)	ZrBr2(g)
CsI(g)	MoBr4(g)	Np(g)	Se(g)	(TeO2)2(g)	ZrBr3(g)
Cs2I2(g)	MoBr5(g)	NpO(g)	Se2(g)	TeOBr2(g)	ZrBr4(g)
CsNa(g)	MoBr6(g)	O2(g)	Se3(g)	U(g)	ZrI(g)
CsO(g)	Mol(g)	Pd(g)	Se4(g)	UBr(g)	ZrI2(g)
Cs2O(g)	Mol2(g)	PdBr2(g)	SeBr2(g)	UBr2(g)	ZrI3(g)
Cs2O2(g)	Mol3(g)	PdO(g)	Se2Br2(g)	UBr3(g)	ZrI4(g)
CsRb(g)	Mol4(g)	Pu(g)	SeO(g)	UBr4(g)	ZrO(g)
Cs2RuO4(g)	Mol5(g)	PuBr3(g)	SeO2(g)	UBr5(g)	ZrO2(g)
Eu(g)	Mol6(g)	PuI3(g)	SeOBr2(g)	UI(g)	ZrTe2(g)

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