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CHEMICAL THERMODYNAMIC MODELING OF MOLTEN SALTS TO SUPPORT OFF-GAS ABATEMENT SYSTEMS

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ORNL IS MANAGED BY UT-BATTELLE LLC FOR THE US DEPARTMENT OF ENERGY

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Nuclear Energy and Fuel Cycle Division

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ABSTRACT

The reprocessing of used nuclear fuel by any means will liberate gaseous fission products, such as hydrogen (^{3}H), carbon (^{14}C), noble gases (^{85}Kr), and halogens (^{129}I), from the irradiated fuel. These elements will distribute through chemical processing operations and partition into process off-gas streams, and the specific volatile release fractions will be dictated by the chemical and physical properties of the system. A recent assessment found that there were significant knowledge gaps regarding the release quantities of volatile radionuclides from individual unit operations. These knowledge gaps limited the ability to determine what dedicated off-gas treatment technologies could be required for electrochemical-based reprocessing facilities. Unfortunately, experimental efforts to quantify release fractions are limited by the challenges associated with performing experiments using irradiated fuel. This report documents preliminary thermodynamic predictions of iodine and tritium release from chloride-based molten salts as part of an effort to better direct resources toward those experiments (both simulant and irradiated) that will be of the greatest impact. It was predicted that less than 0.5% of tritium was expected to be released and that nearly all of that amount would be released as H_2. Thermochemical data for hydrogen (H_2) are of high fidelity, and no additional validation is recommended. Less than 0.05% of iodine was predicted to be released, with the primary volatile species being Cs_2I_2. Unlike the tritium predictions, the data underpinning the iodine release predictions are of low quality. It is recommended that a limited experimental program be dedicated to expanding the current physical property and thermodynamic property data for iodine in electrochemical processing and molten salt conditions, including vapor pressure measurements for the dimerized species predicted to comprise the majority of iodine release. Validating and improving the thermodynamic properties used in predictive modeling can reduce the need for expensive testing with irradiated fuel.

1. INTRODUCTION

The reprocessing of used nuclear fuel by any means will liberate gaseous fission products from the irradiated fuel. Potential volatile elements with isotopes of concern include hydrogen (^{3}H), carbon (^{14}C), noble gases (^{85}Kr), and halogens (^{129}I), and these elements will distribute through chemical processing operations based on their individual chemical speciation and physical properties. Many of these volatile radionuclides (RNs) will partition into the off-gas streams associated with fuel reprocessing. These off-gas streams arise from multiple sources, such as the sparging of liquids or molten salts, venting of process vessels, and sweeping or blanketing of operations conducted in an inert environment. Any venting of RN-bearing process gas streams to the environment is governed by US regulations limiting the emitted radioactivity from nuclear facilities.

The applicable regulations include 40 CFR 190.10, 40 CFR 61, and 10 CFR 20 (EPA 2010a, EPA 2010b, NRC 2012). Extensive technical assessments have been performed to determine how these regulations may be applied to a reprocessing plant that processes used UO_2 fuel by aqueous separations technology; these assessments were developed using detailed understanding of the chemical emissions of the processing technologies, the potential plant design, and the transport or dispersion of volatile RNs that may occur after emission from the facility (Soelberg 2008, Jubin et al. 2012a, Jubin et al. 2012b, Jubin et al. 2013, Jubin et al. 2014, Jubin et al. 2016). A similar assessment was performed more recently for a facility using electrochemical reprocessing techniques to recover uranium from metallic uranium alloy used nuclear fuel (Bruffey et al. 2020). This assessment found that there were significant knowledge gaps regarding the release quantities of volatile RNs from individual unit operations. These knowledge gaps limited the ability to determine what dedicated off-gas treatment technologies could be required for electrochemical-based reprocessing facilities.

An example of this limitation is the characterization of iodine distribution within the initial electrorefining operation. Nearly all the iodine produced during irradiation and found in the spent fuel matrix would be expected to transfer to the electrorefiner. In the electrorefiner, chopped used fuel segments are dissolved into a molten chloride salt (such as LiCl–KCl) at ~500°C under an applied potential. There are several iodine species that could be formed upon fuel dissolution; iodine will exist as an anion and could complex with many different elements present within the fuel, including other halides (e.g., ICl_3) and group 1 elements (e.g., KI). It may also exist as the volatile species I_2. However, the proportion of iodine existing in volatile and non-volatile forms is not known with high precision. Experimental efforts have been performed on irradiated fuel to quantify iodine release during the unit operations of electrochemical processing (Frank, 2011), but the measurement errors produce an uncertainty of greater than 5%, which is at least an order of magnitude higher than the level of precision required to assess the source term from an off-gas perspective.

Unfortunately, experimental efforts to better understand the iodine release fraction from the electrorefiner or from other operations is limited by the challenges associated with performing experiments using irradiated fuel. This is also true for the other volatile species that could be present within the electrochemical processing flowsheet (most notably, tritium). As part of an effort to better direct resources toward those experiments (both simulant and irradiated) that will be of greatest impact, this report documents the performed preliminary thermodynamic predictions of iodine and tritium release from chloride-based molten salts.

Although there are some existing thermodynamic computational packages available, including advanced Gibbs energy minimization (GEM) software, this review is put forth at a time when the resurgence of molten salt nuclear reactor designs has catalyzed many research efforts devoted to the development of new chemical and thermodynamic databases intended to improve the understanding of salt behavior. There will be many common chemical phenomena or challenges shared by both molten salt reactors and pyroprocessing, which is conducted in a molten salt bath. Therefore, it was important to ensure that the current state of knowledge surrounding molten salt modeling was taken into account and that its applicability—as well as the applicability of existing computational resources—was understood.

This effort surveyed available thermodynamic modeling resources, performed initial thermodynamic predictions for iodine and tritium release from molten salts, and then assessed the fidelity of the underlying data to better direct future R&D associated with the management of pyroprocessing off-gases.

2. MOLTEN SALT THERMODYNAMIC MODELING

Thermodynamic modeling efforts informed by updated speciation and physical property data in the context of the MSR are ongoing, and it is likely that some of these efforts will provide advancements that could be leveraged to better understand electrochemical processing systems. Some notable efforts include the following works.

Ard et al. (2019) detail the use of the calculation of phased diagram (CALPHAD) approach to develop a Molten Salt Thermodynamic Database (MSTDB) that accounts for fission and activation products etc. This method relies on the calculation of Gibbs free energy within the system to determine stability of each constituent within the salt solution.

Greenwood et al. (2020) seeks to integrate chemistry capabilities into the Transient Simulation Framework of Reconfigurable Models (TRANSFORM) and couple this with (MSTDB). Ultimately, this may lead to more accurate mass accountancy with the ability to track species across as many process operations as can be programmed into the model.

In consideration of the effects of corrosion and the removal and deposition material in contact with a fluid salt, the Yellowjacket corrosion suite simulates leaching (NEAMS). It relies on thermophysical properties as a basis for mass accountancy. The code suite comprises (Graham 2020):

- "Yellowjacket," a mesoscale phase field (PF) code for corrosion
- "Mole," an engineering scale diffusion, and reaction kinetics code
- A GEM with an accompanying thermodynamic database (MSTDB-TC). The GEM is part of Yellowjacket.
- A database for prediction of thermophysical properties (MSTDB-TP) derived from simulations and available experiments (performed by other programs).

After reviewing the relevant literature and consulting with molten salt chemistry experts, the FactSage Thermodynamic database and GEM were selected as a starting point for the thermodynamic calculations performed in this report. This approach provides consistency with McMurray et al. (2018). FactSage provides access to both solution databases and compound databases. The former database contains optimized model parameters for the Gibbs energy of solution phases as functions of composition and temperature. The latter database contains the properties of stoichiometric compounds (pure substances), either obtained from published experimental data and phase diagram optimizations or taken from standard compilations. (General Compound Databases)

3. CALCULATION OF THERMODYNAMIC EQUILIBRIUM

To better understand the vapor behavior of iodine and tritium within the salt, thermodynamic calculations using FactSage were performed.

3.1 ASSUMPTIONS

A full understanding the transfer rate of volatile species from the molten salt dissolved fuel mixture would encompass the knowledge of the gas-salt equilibria as well as mass transfer rates for each species. The evolution of gaseous species from the salt in the electrorefining cell can be approximated as a static molten salt bed whose vapor head space is open to the glove box in which it is contained. Consideration of movement of species as a function of diffusion or electrochemical potential is omitted; only unidirectional transport is considered. Figure 1 gives an illustration of the proposed system.

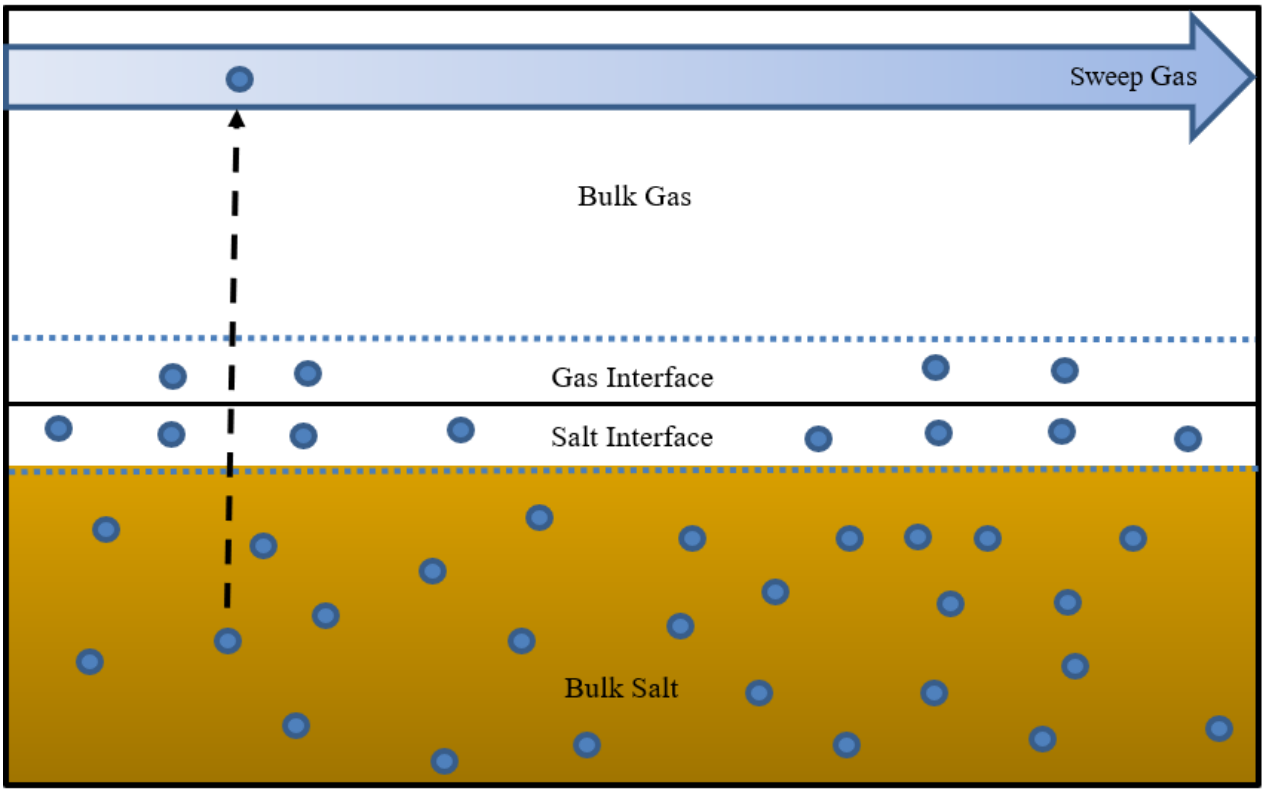

Figure 1. Illustration describing the proposed transfer of volatile species from the fuel-salt solution to the headspace and removal by sweep gas.

The assumption that it is static (no stirring or mixing) means that the transport from the bulk salt to the gas-salt interface is driven entirely by differences in chemical potential as opposed to convection. Equation 1 shows a representation of the mass transfer from the salt to the interface, were $d(m_i)/dt$ is the rate of transfer over time, k is the mass transfer coefficient, A is the interfacial cross-sectional area, and $C_{x,\,i}$ are the concentrations of species i at the relevant locations (bulk salt, interface, or bulk gas) denoted as x.

$$\frac{d(m_i)}{dt} = k_{Salt} A(C_{salt,bulk,\,i} - C_{salt,interface,\,i}) \quad (\mathbf{1})$$

Because of the high temperatures, the transport from the bulk salt to the salt interface is assumed to be extremely rapid such that the difference between the two concentrations is very small ($C_{salt,bulk,i} \approx C_{salt,interface,i}$). In the gas phase, the corresponding transport equation can be represented via Eq. (2).

$$\frac{d(m_i)}{dt} = k_{gas} A(C_{gas,\,interface,i} - C_{gas,\,bulk,i}) \quad (\mathbf{2})$$

This framework is derived from the work done by Greenwood et al. (2020). However, in this work's system of interest, the presence of a sweep gas that constantly dilutes and removes volatile species from the headspace allows for the additional assumption that the headspace is sufficiently dilute such that the concentration in the bulk gas is assumed to be negligible.

$$\frac{d(m_i)}{dt} = k_{gas} A C_{gas,\, interface,i} \tag{3}$$

Finally, it was assumed that there is no accumulation of volatile RN species at the interface, meaning that the rate of transfer from the salt-side interfacial film to the interface is equal to the rate of transfer from gas-side film to the bulk gas.

To proceed with the equations listed above, both the species of interest that are found within the dissolved spent fuel molten salt solution as well as their quantities (relative to some fuel amount, composition, burn-up, cooling etc.,) must first be established.

For an estimation of the species and their quantities, we used data taken from the FactSage Equilibrium simulation software. Within this, the FactPS (Pure Substance) database houses Gibbs free energy data for roughly 5,000 chemical species in various phases. The FactSage Equilibrium calculation software was used to determine the theoretical concentrations by performing a GEM. It is assumed that under high operating temperature and low pressure, there is very little deviation between the real gases and ideal gases; therefore, the ideal gas equation of state was used.

3.2 INPUTS AND SIMULATION RESULTS

The composition of the spent fuel used in this simulation example can be found in Table A-1. This composition does not include any cladding, plenum, duct, or other non-fuel masses. The metallic uranium fuel selected as the source term is assumed to be alloyed with zirconium and plutonium and to be at equilibrium within a closed fuel cycle with a conversion ratio of 0.75. Initial fuel composition is assumed to be 70 wt% U–20 wt% TRU–10 wt% Zr. The equilibrium composition of the TRU components of the used fuel for the system with a conversion ratio of 0.75 is 0.21% Np–17.7 wt% Pu–0.92 wt% Am–0.38 wt% Cm. The FactPS database was unable to provide information on Cf, Cm, Pa, Bk, and Ac; therefore, the results do not account for the presence of these species in the dissolved salt matrix. Similarly, because FactSage Equilibrium is capable of simulating only 48 species at a time, Fr and Po were omitted because they present in the lowest quantity. Bruffey et al. (2020) suggests a dissolution ratio of 3–8 wt% of U in LiCl-KCl (44.3% mol LiCl and 55.7% mol KCl). For the simulation inputs herein, a midpoint value of 5.5 wt% U dissolved in the salt based on the arithmetic mean of the range was specified, given in Bruffey et al. The total mass of salt was then calculated based on the total mass of U in the fuel inventory such that it yielded the 5.5 wt% in salt.

The composition of the resulting gas phase in equilibrium with the salt-fuel mixture at 500°C can be seen in Appendix A-2 along with results for the mole fraction of the off-gas occupied by iodine and hydrogen species. By subtracting the moles of both hydrogen and iodine released as various compounds in the gas phase from the initial moles in the fuel inventory, and accounting for stoichiometry, the simulation predicts a 0.03% release for iodine and 0.42% for hydrogen. Figures 2 and 3 show which chemical species are predicted to contribute to this small release fraction.

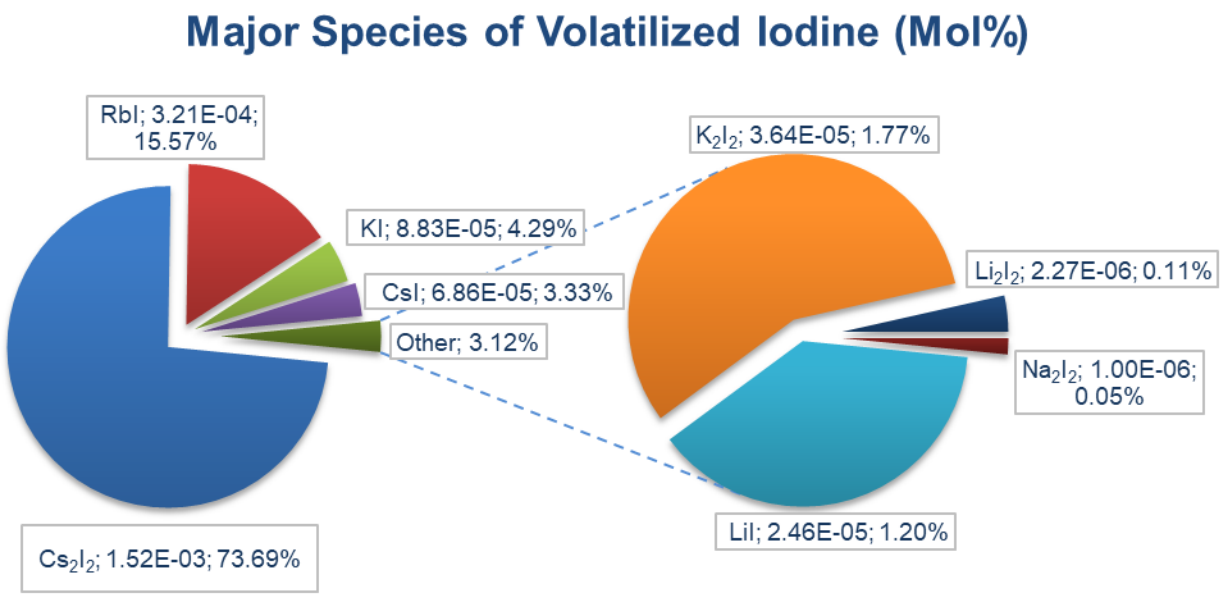

Figure 2. Total iodine released broken down by species. Numbers in parentheses represent moles and mole percent per assembly dissolved.

Table 1: Iodine release data. Per the composition specifications of Bruffey and fellows (Bruffey 2020), the Iodine isotopes under consideration are ^{127}I (25%) and ^{129}I (75%). The activity represented here reflects only that of unstable ^{129}I and does not include any contribution from radioactive cations. The molar and mass quantities reflect the sum of both isotopes.

Species	I-129 Activity (Ci)/MTIHM	Moles/MTIHM	Mass (g)/MTIHM
Cs_2I_2	2.59E-05	1.52E-03	1.95E-01
RbI	5.46E-06	3.21E-04	4.12E-02
KI	1.50E-06	8.83E-05	1.13E-02
CsI	1.17E-06	6.86E-05	8.82E-03
LiI	4.20E-07	2.46E-05	3.16E-03
K_2I_2	6.20E-07	3.64E-05	4.68E-03
Li_2I_2	3.86E-08	2.27E-06	2.91E-04
Na_2I_2	1.70E-08	1.00E-06	1.28E-04

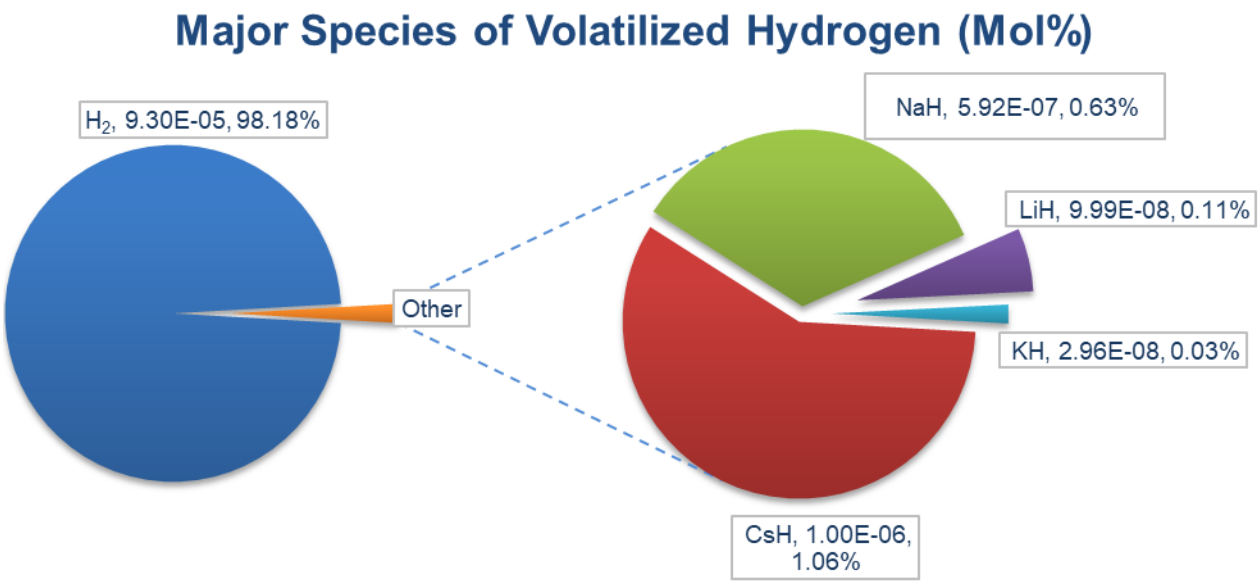

Table 2: Tritium release data. Activities reflect only the tritium contribution.

Species	Tritium Activity (Ci)/MTIHM	Moles/MTIHM	Mass (g)/MTIHM
H_2	2.70E+00	9.30E-05	2.79E-04
CsH	2.90E-02	1.00E-06	3.00E-06
NaH	1.72E-02	5.92E-07	1.78E-06
LiH	2.89E-03	9.99E-08	3.00E-07
KH	8.59E-04	2.96E-08	8.89E-08

Figure 3. Total hydrogen released broken down by species. Numbers in parentheses represent moles and mole percent per assembly dissolved.

Though there are several more species present in the headspace gas, those that are not present in Figures 2 and 3 are assumed to be negligible and will not be discussed here further. Amounts for these can be found in Table A-2.

The dimerization of several iodine species was predicted by the simulation, particularly Cs_2I_2, which appears to be the dominant volatilized iodine species. Its monomeric form appears with approximately 22× less prevalence. The dimerization of gas phase Cs_2I_2 was discussed by Cordfunke (1986).

4. DATA NEEDS AND PATH FORWARD

As with any computational effort, benchmarking and data fidelity are critical to ensuring the validity of the results.

In this case, it was found that the hydrogen release is predicted to occur nearly completely (98.2%) as H_2. The authors suggest that the remaining hydrogen-bearing constituents be treated as negligible in the gas

phase modelling and that the parameters required are only those of hydrogen, which are readily available and have a high level of precision and validation.

The thermodynamic parameters required to support vapor-phase iodine predictions were less well understood. The vapor pressures of many of the iodine-containing compounds of interest cannot be reliably determined using Antoine's equation because the operational temperature is beyond the recommended range. It may be necessary to apply the Clausius–Clapeyron equation to extrapolate the vapor pressure from the available interval to 500°C, which is below the lower bound. Obtaining key data, such as the heats of vaporization of the dimer species, as well as the necessary Antoine parameters and relevant temperature ranges, would be impactful to modeling not just this system, but also to understanding possible vapor phase iodine speciation and partial pressures in the headspace of molten salt reactors. Table 1 shows the data available for simple salts and the lack of data for dimerized salts.

Table 3: Physical properties of key iodine-based salts

Species	ΔH_{vap} (kJ mol^{-1})	T_{vap} (K)	A	B	C	T_{min}(°C)	T_{max}(°C)
Cs_2I_2	-	-	-	-	-	-	-
RbI	197.08	1573.15	7.66	7039.85	170.51	748	1300
KI	190.90	1618.00	6.57	5053.29	22.89	745	1344.85
CsI	150.20	1553.15	7.64	6849.98	158.37	738	1280.00
LiI	167.29	1447.00	8.49	7459.86	155.24	723	1173.85
K_2I_2	-	-	-	-	-	-	-
L_2I_2	-	-	-	-	-	-	-
Na_2I_2	-	-	-	-	-	-	-

It is recommended that a limited experimental program be dedicated to expanding the current physical property and thermodynamic property data for iodine in electrochemical processing and molten salt conditions. The temperature ranges over which validated data are required for both simple and dimerized salts are expansive, taking into account electrorefining, high-temperature vacuum distillation processes, normal molten salt reactor operating conditions, and unexpected high-temperature reactor events. This physical and thermodynamic data should include the following:

- Henry's constants and vapor pressure data — to understand the equilibrium relationship between the gaseous species and the salt fluid.
- Sieverts' constants — for the solubility of gaseous species in the metal vessels.
- Mass transfer coefficients — for fewer assumptions to be needed in modeling the transfer rate of gaseous species from the bulk salt to the bulk gas. Needed to fully describe the transport/concentration profile of salt constituents.

The authors suggest that some of these data are easily obtained through the use of existing specialized instrumentation. Tests with iodine-bearing molten salts should be performed to determine the partial pressures exerted across wide temperature ranges, and those headspace gases should be analyzed through close-coupled mass spectrometry to determine the chemical speciation of the volatilized iodine. This type of effort will allow an understanding of iodine release rates from molten salts, validate this thermochemical prediction, and could avoid the requirement to do costly hot-cell validation of iodine release rates from electrochemical fuel processing.

5. ACKNOWLEDGEMENTS

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APPENDIX A. SUPPORTING TABLES

A-1. INITIAL FUEL COMPOSITION SFR USED METAL FUEL (99.6 GWD/MTIHM, 2-Y COOLED, 0.75 CONVERSION RATIO). ADAPTED FROM LAW ET AL. 2015.

Isotope	H3	TOTAL
Mass g/MTIHM	2.28E-01	2.28E-01
Mols/MTIHM	2.28E-02	2.28E-02
Fraction	1.00E+00	1.00E+00

Isotope	C12	C14	TOTAL
Mass g/MTIHM	1.75E+02	0.00E+00	1.75E+02
Mols/MTIHM	1.46E+01	0.00E+00	1.46E+01
Fraction	1.00E+00	0.00E+00	1.00E+00

Isotope	NA	TOTAL
Mass g/MTIHM	2.40E+04	2.40E+04
Mols/MTIHM	1.04E+03	1.04E+03
Fraction	1.00E+00	1.00E+00

Isotope	SE76	SE77	SE78	SE79	SE80	SE81	TOTAL
Mass g/MTIHM	3.85E-02	3.18E+00	6.83E+00	1.20E+01	1.98E+01	5.41E+01	9.59E+01
Mols/MTIHM	5.07E-04	4.13E-02	8.76E-02	1.52E-01	2.48E-01	6.60E-01	1.19E+00
Fraction	4.26E-04	3.47E-02	7.37E-02	1.28E-01	2.08E-01	5.55E-01	1.00E+00

Isotope	KR80	KR81	KR82	KR83	KR84	KR85	KR86	TOTAL
Mass g/MTIHM	9.25E-04	4.06E-05	2.04E+00	1.15E+02	2.09E+02	3.87E+01	3.23E+02	6.88E+02
Mols/MTIHM	1.16E-05	5.01E-07	2.49E-02	1.39E+00	2.49E+00	4.55E-01	3.76E+00	8.11E+00
Fraction	1.43E-06	6.18E-08	3.07E-03	1.71E-01	3.07E-01	5.61E-02	4.63E-01	1.00E+00

Isotope	RB85	RB86	TOTAL

Mass g/MTIHM	1.89E+02	4.25E+02	6.14E+02
Mols/MTIHM	2.22E+00	4.89E+00	7.11E+00
Fraction	3.13E-01	6.87E-01	1.00E+00

Isotope	**SR86**	**SR87**	**SR88**	**SR89**	**SR90**	**TOTAL**
Mass g/MTIHM	7.19E+00	1.42E-01	5.53E+02	1.34E-03	7.74E+02	1.33E+03
Mols/MTIHM	8.36E-02	1.63E-03	6.28E+00	1.51E-05	8.60E+00	1.50E+01
Fraction	5.59E-03	1.09E-04	4.20E-01	1.01E-06	5.75E-01	1.00E+00

Isotope	**Y 89**	**Y 90**	**Y 91**	**TOTAL**
Mass g/MTIHM	7.26E+02	1.94E-01	8.52E-03	7.26E+02
Mols/MTIHM	8.16E+00	2.16E-03	9.36E-05	8.16E+00
Fraction	1.00E+00	2.64E-04	1.15E-05	1.00E+00

Isotope	**ZR 90**	**ZR 91**	**ZR 92**	**ZR 93**	**ZR 94**	**ZR 95**	**ZR 96**	**TOTAL**
Mass g/MTIHM	9.38E+01	1.13E+05	1.22E+03	1.50E+03	1.73E+03	3.70E-02	1.99E+03	1.20E+05
Mols/MTIHM	1.04E+00	1.24E+03	1.33E+01	1.61E+01	1.84E+01	3.89E-04	2.07E+01	1.31E+03
Fraction	7.95E-04	9.47E-01	1.01E-02	1.23E-02	1.40E-02	2.97E-07	1.58E-02	1.00E+00

Isotope	**NB 93**	**NB 93M**	**NB 94**	**NB 95**	**NB 95M**	**TOTAL**
Mass g/MTIHM	5.60E-04	2.68E-03	7.96E-03	4.46E-02	2.66E-05	5.58E-02
Mols/MTIHM	6.02E-06	2.88E-05	8.47E-05	4.69E-04	2.80E-07	5.89E-04
Fraction	1.02E-02	4.89E-02	1.44E-01	7.97E-01	4.75E-04	1.00E+00

Isotope	**MO 95**	**MO 96**	**MO 97**	**MO 98**	**MO100**	**TOTAL**

Mass g/MTIHM	1.87E+03	5.72E+01	2.09E+03	2.35E+03	2.69E+03	9.06E+03
Mols/MTIHM	1.97E+01	5.96E-01	2.15E+01	2.40E+01	2.72E+01	9.30E+01
Fraction	2.12E-01	6.41E-03	2.32E-01	2.58E-01	2.92E-01	1.00E+00

Isotope	**TC 98**	**TC 99**	**TOTAL**
Mass g/MTIHM	0.00E+00	2.39E+03	2.39E+03
Mols/MTIHM	0.00E+00	2.41E+01	2.41E+01
Fraction	0.00E+00	1.00E+00	1.00E+00

Isotope	**RU 99**	**RU100**	**RU101**	**RU102**	**RU103**	**RU104**	**RU106**	**TOTAL**
Mass g/MTIHM	3.28E-02	1.05E+02	2.53E+03	3.07E+03	2.74E-04	2.77E+03	1.43E+02	8.62E+03
Mols/MTIHM	3.31E-04	1.05E+00	2.50E+01	3.01E+01	2.66E-06	2.66E+01	1.36E+00	8.42E+01
Fraction	3.94E-06	1.25E-02	2.98E-01	3.57E-01	3.16E-08	3.16E-01	1.62E-02	1.00E+00

Isotope	**RH102**	**RH103**	**RH103M**	**RH106**	**TOTAL**
Mass g/MTIHM	0.00E+00	2.96E+03	2.70E-07	1.34E-04	2.96E+03
Mols/MTIHM	0.00E+00	2.87E+01	2.62E-09	1.26E-06	2.87E+01
Fraction	0.00E+00	1.00E+00	9.12E-11	4.40E-08	1.00E+00

Isotope	**PD104**	**PD105**	**PD106**	**PD107**	**PD108**	**PD110**	**TOTAL**
Mass g/MTIHM	1.73E-02	2.03E+03	1.94E+03	1.20E+03	1.01E+03	2.75E+02	6.46E+03
Mols/MTIHM	1.66E-04	1.93E+01	1.83E+01	1.12E+01	9.35E+00	2.50E+00	6.07E+01
Fraction	2.74E-06	3.18E-01	3.02E-01	1.85E-01	1.54E-01	4.12E-02	1.00E+00

Isotope	AG107	AG108	AG108M	AG109	AG109M	AG110	AG110M	TOTAL
Mass g/MTIHM	5.50E-04	3.59E-14	1.32E-05	6.45E+02	9.70E-14	1.28E-09	8.09E-02	6.45E+02
Mols/MTIHM	5.14E-06	3.32E-16	1.22E-07	5.92E+00	8.90E-16	1.16E-11	7.35E-04	5.92E+00
Fraction	8.69E-07	5.62E-17	2.07E-08	1.00E+00	1.50E-16	1.97E-12	1.24E-04	1.00E+00

Isotope	CD108	CD109	CD110	CD111	CD112	CD113	CD113M	CD114	CD115M	CD116	TOTAL
Mass g/MTIHM	2.62E-05	9.60E-08	6.01E+01	1.43E+02	9.95E+01	5.10E+01	2.92E+00	4.71E+01	2.21E-06	2.83E+01	4.32E+02
Mols/MTIHM	2.43E-07	8.81E-10	5.46E-01	1.29E+00	8.88E-01	4.51E-01	2.58E-02	4.13E-01	1.92E-08	2.44E-01	3.86E+00
Fraction	6.29E-08	2.28E-10	1.42E-01	3.34E-01	2.30E-01	1.17E-01	6.70E-03	1.07E-01	4.98E-09	6.32E-02	1.00E+00

Isotope	IN113	IN113M	IN114	IN114M	IN115	TOTAL
Mass g/MTIHM	5.70E-01	0.00E+00	8.15E-13	5.03E-08	3.32E+01	3.38E+01
Mols/MTIHM	5.04E-03	0.00E+00	7.15E-15	4.41E-10	2.89E-01	2.94E-01
Fraction	1.72E-02	0.00E+00	2.43E-14	1.50E-09	9.83E-01	1.00E+00

Isotope	SN114	SN115	SN116	SN117	SN118	SN119	SN119M	SN120	SN121M	SN122	SN123	SN124	SN126	TOTAL
Mass g/MTIHM	1.50E-02	1.11E+00	2.48E+00	2.78E+01	2.98E+01	2.84E+01	2.86E-02	2.96E+01	6.13E-02	3.33E+01	4.29E-02	5.29E+01	1.30E+02	3.36E+02
Mols/MTIHM	1.32E-04	9.65E-03	2.14E-02	2.38E-01	2.53E-01	2.39E-01	2.40E-04	2.47E-01	5.07E-04	2.73E-01	3.49E-04	4.27E-01	1.03E+00	2.74E+00
Fraction	4.80E-05	3.52E-03	7.81E-03	8.67E-02	9.22E-02	8.71E-02	8.77E-05	9.01E-02	1.85E-04	9.97E-02	1.27E-04	1.56E-01	3.77E-01	1.00E+00

Isotope	SB121	SB123	SB124	SB125	SB126	SB126M	TOTAL
Mass g/MTIHM	3.03E+01	3.96E+01	3.04E-05	3.16E+01	6.16E-06	4.69E-08	1.02E+02
Mols/MTIHM	2.50E-01	3.22E-01	2.45E-07	2.53E-01	4.89E-08	3.72E-10	8.25E-01
Fraction	3.03E-01	3.90E-01	2.97E-07	3.06E-01	5.92E-08	4.51E-10	1.00E+00

Isotope	TE122	TE123	TE123M	TE124	TE125	TE125M	TE126	TE127	TE127M	TE128	TE129	TE129M	TE130	TOTAL
Mass g/MTIHM	1.20E+00	1.73E-02	2.14E-05	1.40E+00	5.63E+01	4.43E-01	7.29E+00	1.30E-04	3.71E-02	4.12E+02	1.24E-09	1.34E-06	1.23E+03	1.71E+03
Mols/MTIHM	9.84E-03	1.41E-04	1.74E-07	1.13E-02	4.50E-01	3.54E-03	5.79E-02	1.02E-06	2.92E-04	3.22E+00	9.61E-12	1.04E-08	9.46E+00	1.32E+01
Fraction	7.44E-04	1.06E-05	1.32E-08	8.54E-04	3.41E-02	2.68E-04	4.38E-03	7.75E-08	2.21E-05	2.44E-01	7.27E-13	7.86E-10	7.16E-01	1.00E+00

Isotope	I127	I129	TOTAL
Mass g/MTIHM	2.49E+02	7.53E+02	1.00E+03
Mols/MTIHM	1.96E+00	5.84E+00	7.80E+00
Fraction	2.51E-01	7.49E-01	1.00E+00

Isotope	XE128	XE129	XE130	XE131	XE132	XE134	XE136	TOTAL
Mass g/MTIHM	1.47E+01	1.03E-01	1.35E+00	2.08E+03	2.98E+03	3.99E+03	3.68E+03	1.27E+04
Mols/MTIHM	1.15E-01	7.98E-04	1.04E-02	1.59E+01	2.26E+01	2.98E+01	2.71E+01	9.54E+01
Fraction	1.20E-03	8.37E-06	1.09E-04	1.66E-01	2.37E-01	3.12E-01	2.84E-01	1.00E+00

Isotope	CS133	CS134	CS135	CS137	TOTAL
Mass g/MTIHM	3.61E+03	4.67E+01	4.08E+03	3.42E+03	1.12E+04
Mols/MTIHM	2.71E+01	3.49E-01	3.02E+01	2.50E+01	8.27E+01
Fraction	3.28E-01	4.22E-03	3.66E-01	3.02E-01	1.00E+00

Isotope	BA134	BA135	BA136	BA137	BA137M	BA138	TOTAL
Mass g/MTIHM	9.95E+01	7.20E-02	1.78E+02	3.59E+02	5.21E-04	3.69E+03	4.33E+03
Mols/MTIHM	7.43E-01	5.33E-04	1.31E+00	2.62E+00	3.80E-06	2.67E+01	3.14E+01
Fraction	2.36E-02	1.70E-05	4.17E-02	8.34E-02	1.21E-07	8.51E-01	1.00E+00

Isotope	LA138	LA139	TOTAL
Mass g/MTIHM	5.11E-03	3.39E+03	3.39E+03
Mols/MTIHM	3.70E-05	2.44E+01	2.44E+01

Fraction	1.52E-06	1.00E+00	1.00E+00	

Isotope	**CE140**	**CE142**	**CE144**	**TOTAL**
Mass g/MTIHM	3.19E+03	2.81E+03	8.85E+01	6.09E+03
Mols/MTIHM	2.28E+01	1.98E+01	6.15E-01	4.32E+01
Fraction	5.28E-01	4.58E-01	1.42E-02	1.00E+00

Isotope	**PR141**	**PR144**	**PR144M**	**TOTAL**
Mass g/MTIHM	3.26E+03	3.74E-03	1.87E-05	3.26E+03
Mols/MTIHM	2.31E+01	2.60E-05	1.30E-07	2.31E+01
Fraction	1.00E+00	1.12E-06	5.62E-09	1.00E+00

Isotope	**ND142**	**ND143**	**ND144**	**ND145**	**ND146**	**ND148**	**ND150**	**TOTAL**
Mass g/MTIHM	2.89E+01	2.57E+03	2.35E+03	1.77E+03	1.78E+03	1.07E+03	6.47E+02	1.02E+04
Mols/MTIHM	2.04E-01	1.80E+01	1.63E+01	1.22E+01	1.22E+01	7.23E+00	4.31E+00	7.04E+01
Fraction	2.89E-03	2.55E-01	2.32E-01	1.73E-01	1.73E-01	1.03E-01	6.12E-02	1.00E+00

Isotope	**PM147**	**PM148**	**PM148M**	**TOTAL**
Mass g/MTIHM	4.10E+02	1.67E-07	1.86E-05	4.10E+02
Mols/MTIHM	2.79E+00	1.13E-09	1.26E-07	2.79E+00
Fraction	1.00E+00	4.05E-10	4.51E-08	1.00E+00

Isotope	**SM146**	**SM147**	**SM148**	**SM149**	**SM150**	**SM151**	**SM152**	**SM154**	**TOTAL**
Mass g/MTIHM	0.00E+00	7.79E+02	1.74E+02	7.96E+02	1.11E+02	4.53E+02	4.82E+02	1.92E+02	2.99E+03
Mols/MTIHM	0.00E+00	5.30E+00	1.18E+00	5.34E+00	7.40E-01	3.00E+00	3.17E+00	1.25E+00	2.00E+01
Fraction	0.00E+00	2.65E-01	5.89E-02	2.67E-01	3.70E-02	1.50E-01	1.59E-01	6.24E-02	1.00E+00

Isotope	**EU150**	**EU151**	**EU152**	**EU153**	**EU154**	**EU155**	**TOTAL**

Mass g/MTIHM	0.00E+00	1.38E+01	5.29E-01	2.28E+02	2.54E+01	7.85E+01	3.46E+02	
Mols/MTIHM	0.00E+00	9.14E-02	3.48E-03	1.49E+00	1.65E-01	5.06E-01	2.26E+00	
Fraction	0.00E+00	4.05E-02	1.54E-03	6.60E-01	7.31E-02	2.24E-01	1.00E+00	

Isotope	**GD152**	**GD153**	**GD154**	**GD155**	**GD156**	**GD157**	**GD158**	**GD160**	**TOTAL**
Mass g/MTIHM	3.98E-01	3.14E-04	8.82E+00	5.98E+01	1.08E+02	5.81E+01	5.24E+01	1.44E+01	3.02E+02
Mols/MTIHM	2.62E-03	2.05E-06	5.73E-02	3.86E-01	6.92E-01	3.70E-01	3.32E-01	9.00E-02	1.93E+00
Fraction	1.32E-03	1.04E-06	2.92E-02	1.98E-01	3.58E-01	1.92E-01	1.74E-01	4.77E-02	1.00E+00

Isotope	**TB159**	**TB160**	**TOTAL**
Mass g/MTIHM	2.21E+01	4.01E-04	2.21E+01
Mols/MTIHM	1.39E-01	2.51E-06	1.39E-01
Fraction	1.00E+00	1.80E-05	1.00E+00

Isotope	**HO165**	**HO166M**	**TOTAL**
Mass g/MTIHM	5.09E-01	9.05E-04	5.10E-01
Mols/MTIHM	3.08E-03	5.45E-06	3.09E-03
Fraction	9.98E-01	1.76E-03	1.00E+00

Isotope	**TL207**	**TL208**	**TL209**	**TOTAL**
Mass g/MTIHM	1.33E-14	7.28E-10	2.06E-16	7.28E-10
Mols/MTIHM	6.43E-17	3.50E-12	9.86E-19	3.50E-12
Fraction	1.84E-05	1.00E+00	2.82E-07	1.00E+00

Isotope	**PB206**	**PB207**	**PB208**	**PB209**	**PB210**	**PB211**	**PB212**	**PB214**	**TOTAL**
Mass g/MTIHM	9.50E-12	2.02E-09	5.95E-04	8.44E-13	2.28E-10	1.02E-13	4.23E-07	8.04E-15	5.95E-04
Mols/MTIHM	4.61E-14	9.76E-12	2.86E-06	4.04E-15	1.09E-12	4.83E-16	2.00E-09	3.76E-17	2.86E-06
Fraction	1.61E-08	3.41E-06	9.99E-01	1.41E-09	3.79E-07	1.69E-10	6.97E-04	1.31E-11	1.00E+00

Isotope	**BI209**	**BI210**	**BI211**	**BI212**	**BI213**	**BI214**	**TOTAL**

Mass g/MTIHM	1.28E-07	1.49E-13	6.10E-15	4.03E-08	2.04E-13	5.91E-15	1.68E-07
Mols/MTIHM	6.12E-10	7.10E-16	2.89E-17	1.90E-10	9.58E-16	2.76E-17	8.03E-10
Fraction	7.63E-01	8.84E-07	3.60E-08	2.37E-01	1.19E-06	3.44E-08	1.00E+00

Isotope	**PO210**	**PO216**	**PO218**	**TOTAL**
Mass g/MTIHM	3.23E-12	1.69E-12	9.32E-16	4.92E-12
Mols/MTIHM	1.54E-14	7.82E-15	4.28E-18	2.32E-14
Fraction	6.63E-01	3.37E-01	1.84E-04	1.00E+00

Isotope	**RN219**	**RN220**	**RN222**	**TOTAL**
Mass g/MTIHM	1.96E-16	6.44E-10	1.71E-12	6.46E-10
Mols/MTIHM	8.95E-19	2.93E-12	7.70E-15	2.93E-12
Fraction	3.05E-07	9.97E-01	2.62E-03	1.00E+00

Isotope	**FR221**	**FR223**	**TOTAL**
Mass g/MTIHM	2.16E-14	9.20E-16	2.25E-14
Mols/MTIHM	9.77E-17	4.13E-18	1.02E-16
Fraction	9.59E-01	4.05E-02	1.00E+00

Isotope	**RA223**	**RA224**	**RA225**	**RA226**	**RA228**	**TOTAL**
Mass g/MTIHM	4.92E-11	3.68E-06	9.78E-11	2.67E-07	9.32E-15	3.95E-06
Mols/MTIHM	2.21E-13	1.64E-08	4.35E-13	1.18E-09	4.09E-17	1.76E-08
Fraction	1.25E-05	9.33E-01	2.47E-05	6.71E-02	2.32E-09	1.00E+00

Isotope	**AC225**	**AC227**	**AC228**	**TOTAL**
Mass g/MTIHM	6.61E-11	3.45E-08	9.72E-19	3.46E-08
Mols/MTIHM	2.94E-13	1.52E-10	4.26E-21	1.52E-10
Fraction	1.93E-03	9.98E-01	2.80E-11	1.00E+00

Isotope	**TH227**	**TH228**	**TH229**	**TH230**	**TH231**	**TH232**	**TH234**	**TOTAL**
Mass g/MTIHM	7.88E-11	7.15E-04	1.79E-05	9.58E-03	1.07E-09	7.25E-05	1.01E-05	1.04E-02
Mols/MTIHM	3.47E-13	3.14E-06	7.82E-08	4.17E-05	4.63E-12	3.13E-07	4.32E-08	4.52E-05

Fraction	7.68E-09	6.93E-02	1.73E-03	9.21E-01	1.02E-07	6.91E-03	9.54E-04	1.00E+00

Isotope	**PA231**	**PA233**	**PA234**	**PA234M**	**TOTAL**
Mass g/MTIHM	4.79E-04	7.09E-05	1.17E-10	3.39E-10	5.50E-04
Mols/MTIHM	2.07E-06	3.04E-07	5.00E-13	1.45E-12	2.38E-06
Fraction	8.72E-01	1.28E-01	2.10E-07	6.09E-07	1.00E+00

Isotope	**U232**	**U233**	**U234**	**U235**	**U236**	**U237**	**U238**	**U240**	**TOTAL**
Mass g/MTIHM	4.49E-02	2.12E-02	6.38E+02	2.64E+02	4.15E+02	2.42E-04	6.99E+05	1.38E-12	7.00E+05
Mols/MTIHM	1.94E-04	9.10E-05	2.73E+00	1.12E+00	1.76E+00	1.02E-06	2.94E+03	5.77E-15	2.94E+03
Fraction	6.58E-08	3.09E-08	9.27E-04	3.82E-04	5.98E-04	3.47E-10	9.98E-01	1.96E-18	1.00E+00

Isotope	**NP237**	**NP239**	**NP240M**	**TOTAL**
Mass g/MTIHM	2.06E+03	3.33E-03	1.19E-14	2.06E+03
Mols/MTIHM	8.69E+00	1.39E-05	4.96E-17	8.69E+00
Fraction	1.00E+00	1.60E-06	5.70E-18	1.00E+00

Isotope	**PU236**	**PU238**	**PU239**	**PU240**	**PU241**	**PU242**	**PU243**	**PU244**	**TOTAL**
Mass g/MTIHM	2.47E-02	4.85E+03	9.39E+04	5.79E+04	8.08E+03	1.23E+04	1.06E-09	7.21E-02	1.77E+05
Mols/MTIHM	1.05E-04	2.04E+01	3.93E+02	2.41E+02	3.35E+01	5.08E+01	4.36E-12	2.95E-04	7.39E+02
Fraction	1.42E-07	2.76E-02	5.32E-01	3.27E-01	4.54E-02	6.88E-02	5.90E-15	4.00E-07	1.00E+00

Isotope	**AM241**	**AM242**	**AM242M**	**AM243**	**AM244**	**TOTAL**
Mass g/MTIHM	4.93E+03	3.48E-03	2.90E+02	4.03E+03	5.60E-17	9.25E+03
Mols/MTIHM	2.05E+01	1.44E-05	1.20E+00	1.66E+01	2.30E-19	3.82E+01
Fraction	5.35E-01	3.76E-07	3.13E-02	4.34E-01	6.00E-21	1.00E+00

Isotope	**CM242**	**CM243**	**CM244**	**CM245**	**CM246**	**CM247**	**CM248**	**TOTAL**

Mass g/MTIHM	1.13E+01	1.93E+01	2.61E+03	7.21E+02	3.83E+02	3.10E+01	1.43E+01	3.79E+03
Mols/MTIHM	4.67E-02	7.94E-02	1.07E+01	2.94E+00	1.56E+00	1.26E-01	5.77E-02	1.55E+01
Fraction	3.01E-03	5.12E-03	6.90E-01	1.90E-01	1.00E-01	8.09E-03	3.72E-03	1.00E+00

Isotope	**BK249**	**TOTAL**
Mass g/MTIHM	5.80E-02	5.80E-02
Mols/MTIHM	2.33E-04	2.33E-04
Fraction	1.00E+00	1.00E+00

Isotope	**CF250**	**CF251**	**CF252**	**TOTAL**
Mass g/MTIHM	1.75E-01	2.34E-02	8.73E-04	1.99E-01
Mols/MTIHM	7.00E-04	9.32E-05	3.46E-06	7.97E-04
Fraction	8.79E-01	1.17E-01	4.35E-03	1.00E+00

A-2. EQUILIBRIUM GAS COMPOSITION.

Species	Mol%	Moles	Species	Mol%	Moles	Species	Mol%	Moles
Xe	8.99E-01	9.54E+01	**(KCl)2**	1.23E-08	1.30E-06	**Tl**	3.30E-14	3.50E-12
Kr	7.64E-02	8.11E+00	**(RbCl)2**	1.18E-08	1.25E-06	**Rn**	2.77E-14	2.93E-12
Rb	7.53E-03	7.99E-01	**NaCl**	1.13E-08	1.19E-06	**InH**	1.82E-14	1.93E-12
Cd	5.69E-03	6.04E-01	**Li2**	1.12E-08	1.19E-06	**Ho**	7.70E-15	8.18E-13
Na	5.33E-03	5.65E-01	**(LiI)2**	1.07E-08	1.13E-06	**BaI2**	4.60E-15	4.88E-13
Cs	3.18E-03	3.37E-01	**CsH**	9.43E-09	1.00E-06	**BaCl2**	4.14E-15	4.39E-13
K	2.55E-03	2.71E-01	**Sm**	6.74E-09	7.15E-07	**InCl**	2.07E-15	2.19E-13
Na2	1.86E-04	1.98E-02	**NaH**	5.58E-09	5.92E-07	**SrCl2**	8.86E-16	9.40E-14
Rb2	2.34E-05	2.48E-03	**Na2I2**	4.71E-09	5.00E-07	**SrI2**	8.85E-16	9.40E-14
Cs2I2	7.15E-06	7.59E-04	**LiH**	9.41E-10	9.99E-08	**H**	6.01E-16	6.38E-14
K2	5.30E-06	5.63E-04	**Na2Cl2**	9.15E-10	9.71E-08	**SrH**	2.63E-16	2.79E-14
Li	4.98E-06	5.28E-04	**KH**	2.79E-10	2.96E-08	**Bi2**	2.52E-16	2.67E-14
Cs2	3.69E-06	3.91E-04	**Ra**	1.66E-10	1.76E-08	**BaH**	1.51E-16	1.61E-14
RbI	3.02E-06	3.21E-04	**Ba**	8.68E-11	9.22E-09	**Nd**	9.57E-17	1.02E-14
CsCl	8.99E-07	9.55E-05	**KSrCl3**	7.20E-11	7.64E-09	**Sr2**	5.70E-18	6.05E-16
KI	8.32E-07	8.83E-05	**In**	1.91E-11	2.03E-09	**Pu**	2.58E-18	2.74E-16
RbCl	6.48E-07	6.88E-05	**Sb2**	1.64E-11	1.74E-09	**Pb**	1.30E-18	1.38E-16
CsI	6.46E-07	6.86E-05	**Pm**	2.58E-12	2.73E-10	**Pr**	7.96E-19	8.45E-17
(LiCl)2	4.91E-07	5.21E-05	**Sb4**	1.57E-12	1.67E-10	**Ag2**	1.00E-19	1.07E-17
H2	4.38E-07	4.65E-05	**Bi**	1.11E-12	1.17E-10	**Tb**	3.80E-20	4.03E-18
Eu	3.99E-07	4.23E-05	**Am**	9.56E-13	1.01E-10	**SbCl**	2.61E-20	2.76E-18
(CsCl)2	2.83E-07	3.00E-05	**SrI**	7.54E-13	8.00E-11	**HCl**	1.68E-20	1.78E-18
LiCl	2.33E-07	2.47E-05	**Ag**	3.26E-13	3.45E-11	**TlI**	1.41E-20	1.50E-18
LiI	2.32E-07	2.46E-05	**Sb**	3.19E-13	3.38E-11	**Gd**	3.97E-21	4.21E-19
(KI)2	1.71E-07	1.82E-05	**BaI**	2.94E-13	3.12E-11	**AgI**	3.16E-21	3.35E-19
KCl	7.68E-08	8.16E-06	**BaCl**	1.28E-13	1.36E-11	**HI**	1.95E-21	2.07E-19
(LiCl)3	4.41E-08	4.68E-06	**SrCl**	1.22E-13	1.29E-11	**I**	1.59E-21	1.69E-19

Sr	1.64E-08	1.74E-06	InI	1.06E-13	1.12E-11	LaCl3	1.11E-21	1.18E-19
Species	**Mol%**	**Moles**	**Species**	**Mol%**	**Moles**	**Species**	**Mol%**	**Moles**
BiI	6.06E-22	6.43E-20	SbTe	1.54E-29	1.63E-27	H2Se	2.38E-33	2.53E-31
Y	2.27E-22	2.41E-20	SrSe	1.21E-29	1.29E-27	H2Te	1.27E-33	1.35E-31
SbH3	2.05E-22	2.18E-20	GdI3	8.13E-30	8.62E-28	YSe	1.15E-33	1.22E-31
Ce	1.44E-22	1.53E-20	In2Te	7.12E-30	7.55E-28	ThCl4	6.76E-34	7.18E-32
TlCl	1.16E-22	1.23E-20	Te	4.37E-30	4.64E-28	YTe	5.53E-34	5.87E-32
La	5.29E-23	5.61E-21	PbI	2.48E-30	2.64E-28	InSe	4.99E-34	5.30E-32
Ba2	4.91E-23	5.21E-21	NdTe	1.15E-30	1.22E-28	BiSe	3.99E-34	4.23E-32
PrCl3	4.76E-23	5.05E-21	InTe	6.42E-31	6.81E-29	La2	3.34E-34	3.54E-32
CeCl3	4.75E-23	5.04E-21	InCl2	5.09E-31	5.40E-29	CeSe	2.46E-34	2.61E-32
CdI	1.59E-23	1.69E-21	Sn	4.63E-31	4.91E-29	CeTe	2.44E-34	2.59E-32
NdCl3	9.91E-24	1.05E-21	PbCl	3.38E-31	3.59E-29	Ce2	2.23E-34	2.37E-32
PbSb	1.51E-24	1.60E-22	NdSe	2.22E-31	2.36E-29	Zr	1.95E-34	2.07E-32
EuTe	1.37E-24	1.46E-22	BiTe	2.10E-31	2.23E-29	SbSe	1.74E-34	1.85E-32
LaI3	3.75E-25	3.98E-23	LaSe	1.62E-31	1.72E-29	CdSe	1.08E-34	1.14E-32
GdCl3	2.91E-25	3.09E-23	Pd	1.28E-31	1.36E-29	PbTe	1.04E-35	1.10E-33
AgCl	1.62E-25	1.72E-23	LaTe	6.29E-32	6.67E-30	ZrI3	3.45E-36	3.66E-34
TbCl3	1.17E-25	1.24E-23	HoTe	3.75E-32	3.98E-30	Se	3.24E-36	3.43E-34
PbH	1.10E-25	1.17E-23	PrTe	2.69E-32	2.86E-30	Pb2	2.74E-36	2.91E-34
BiCl	9.93E-26	1.05E-23	HoSe	2.35E-32	2.49E-30	Rh	2.69E-36	2.85E-34
PrI3	9.81E-26	1.04E-23	PrSe	2.32E-32	2.46E-30	ZrCl3	5.48E-37	5.82E-35
CeI3	3.99E-26	4.24E-24	Th	1.43E-32	1.52E-30	Mo	2.54E-37	2.70E-35
HoCl3	3.17E-26	3.36E-24	ZrCl	1.28E-32	1.36E-30	I2	1.87E-37	1.99E-35
NdI3	2.11E-26	2.23E-24	TbTe	1.00E-32	1.06E-30	SnCl	1.24E-37	1.32E-35
ZrI2	1.79E-26	1.90E-24	GdTe	8.99E-33	9.54E-31	Y2	5.87E-38	6.23E-36
EuSe	1.77E-26	1.87E-24	GdSe	8.87E-33	9.42E-31	PbSe	4.14E-38	4.39E-36
SmTe	4.52E-27	4.79E-25	TbSe	8.15E-33	8.65E-31	Tc	6.77E-39	7.19E-37
U	1.48E-27	1.57E-25	ZrH	4.12E-33	4.37E-31	ThI4	4.34E-40	4.60E-38
SmSe	1.13E-27	1.20E-25	YCl	4.06E-33	4.31E-31	Ru	2.23E-40	2.37E-38

PuCl3	7.18E-28	7.62E-26	**UCl3**	3.79E-33	4.02E-31	**ICl**	3.62E-41	3.84E-39
Cl	2.43E-29	2.58E-27	**ZrCl2**	3.46E-33	3.67E-31	**ZrCl4**	3.46E-41	3.67E-39
Species	**Mol%**	**Moles**	**Species**	**Mol%**	**Moles**	**Species**	**Mol%**	**Moles**
SnTe	2.56E-41	2.71E-39	**ZrI4**	4.19E-47	4.45E-45	**SbI3**	3.81E-53	4.04E-51
PbI2	1.03E-41	1.09E-39	**Cl2**	2.48E-47	2.63E-45	**SbCl3**	2.78E-53	2.95E-51
Nb	2.31E-42	2.45E-40	**SnI2**	2.28E-47	2.42E-45	**BiI3**	7.55E-55	8.01E-53
Tl2Se	1.34E-42	1.42E-40	**Te2**	1.04E-47	1.11E-45	**Se2**	6.79E-55	7.20E-53
UCl4	9.67E-43	1.03E-40	**MoI2**	6.91E-48	7.33E-46	**BiCl3**	7.31E-59	7.75E-57
USe	3.55E-43	3.77E-41	**InCl3**	3.05E-48	3.23E-46	**RhCl2**	4.00E-60	4.24E-58
UTe	3.41E-43	3.62E-41	**SnCl2**	2.94E-48	3.12E-46	**TeCl2**	3.90E-60	4.14E-58
SnSe	2.10E-43	2.23E-41	**UI4**	5.36E-49	5.69E-47	**NbCl4**	1.52E-62	1.62E-60
InI3	4.08E-44	4.33E-42	**InTe2**	7.88E-51	8.36E-49	**MoI3**	1.16E-62	1.23E-60
PbCl2	1.67E-44	1.77E-42	**TeSe**	5.57E-51	5.91E-49	**UCl5**	4.27E-63	4.53E-61
MoI	1.59E-44	1.69E-42	**ZrI**	1.73E-51	1.84E-49	**PbI4**	4.22E-67	4.48E-65
SnH4	4.26E-45	4.52E-43	**Sn2**	2.48E-52	2.63E-50	**SeCl2**	2.15E-69	2.29E-67
PuCl4	2.96E-45	3.14E-43	**Mo2**	6.24E-53	6.63E-51	**Total**	1.00E+00	1.06E+02

A-3. IODINE CONTAINING GAS CONSTITUENTS. PERCENT VOLATILIZED REPRESENTS THE SUM OF MOLES OF IODINE IN THE GAS RELATIVE TO TOTAL MOLES OF IODINE IN THE INITIAL FUEL FOUND IN A1.

Iodine Species	Mol%	Moles of compound	Moles of Iodine	Mol % of all volatilized Iodine
Cs2I2	7.15E-06	7.59E-04	1.52E-03	73.69%
RbI	3.02E-06	3.21E-04	3.21E-04	15.57%
KI	8.32E-07	8.83E-05	8.83E-05	4.29%
CsI	6.46E-07	6.86E-05	6.86E-05	3.33%
LiI	2.32E-07	2.46E-05	2.46E-05	1.20%
(KI)2	1.71E-07	1.82E-05	3.64E-05	1.77%
(LiI)2	1.07E-08	1.13E-06	2.27E-06	0.11%
Na2I2	4.71E-09	5.00E-07	1.00E-06	0.05%
SrI	7.54E-13	8.00E-11	8.00E-11	0.00%
BaI	2.94E-13	3.12E-11	3.12E-11	0.00%
InI	1.06E-13	1.12E-11	1.12E-11	0.00%
BaI2	4.60E-15	4.88E-13	9.76E-13	0.00%
SrI2	8.85E-16	9.40E-14	1.88E-13	0.00%
TlI	1.41E-20	1.50E-18	1.50E-18	0.00%
AgI	3.16E-21	3.35E-19	3.35E-19	0.00%
HI	1.95E-21	2.07E-19	2.07E-19	0.00%
I	1.59E-21	1.69E-19	1.69E-19	0.00%
BiI	6.06E-22	6.43E-20	6.43E-20	0.00%
(CdI)	1.59E-23	1.69E-21	1.69E-21	0.00%
LaI3	3.75E-25	3.98E-23	1.19E-22	0.00%
PrI3	9.81E-26	1.04E-23	3.12E-23	0.00%
CeI3	3.99E-26	4.24E-24	1.27E-23	0.00%
NdI3	2.11E-26	2.23E-24	6.70E-24	0.00%
ZrI2	1.79E-26	1.90E-24	3.80E-24	0.00%
GdI3	8.13E-30	8.62E-28	2.59E-27	0.00%
PbI	2.48E-30	2.64E-28	2.64E-28	0.00%
ZrI3	3.45E-36	3.66E-34	1.10E-33	0.00%
I2	1.87E-37	1.99E-35	3.98E-35	0.00%
ThI4	4.34E-40	4.60E-38	1.84E-37	0.00%

PbI2	1.03E-41	1.09E-39	2.18E-39	0.00%
InI3	4.08E-44	4.33E-42	1.30E-41	0.00%
MoI	1.59E-44	1.69E-42	1.69E-42	0.00%
ZrI4	4.19E-47	4.45E-45	1.78E-44	0.00%
SnI2	2.28E-47	2.42E-45	4.84E-45	0.00%
MoI2	6.91E-48	7.33E-46	1.47E-45	0.00%
UI4	5.36E-49	5.69E-47	2.28E-46	0.00%
ZrI	1.73E-51	1.84E-49	1.84E-49	0.00%
SbI3	3.81E-53	4.04E-51	1.21E-50	0.00%
BiI3	7.55E-55	8.01E-53	2.40E-52	0.00%
MoI3	1.16E-62	1.23E-60	3.69E-60	0.00%
PbI4	4.22E-67	4.48E-65	1.79E-64	0.00%
Total	1.21E-05	1.28E-03	2.06E-03	

Initial I (Mol/MTIHM)	7.80
% Volatilized	0.03%

A-4. HYDROGEN CONTAINING GAS CONSTITUENTS. PERCENT VOLATILIZED REPRESENTS THE SUM OF MOLES OF HYDROGEN IN THE GAS RELATIVE TO TOTAL MOLES OF HYDROGEN IN THE INITIAL FUEL FOUND IN A1.

Hydrogen Species	Mol% in total gas	Moles of compound	Moles of Hydrogen	Mol % of volatilized hydrogen
H2	4.38E-07	4.65E-05	9.30E-05	98.18%
CsH	9.43E-09	1.00E-06	1.00E-06	1.06%
NaH	5.58E-09	5.92E-07	5.92E-07	0.63%
LiH	9.41E-10	9.99E-08	9.99E-08	0.11%
KH	2.79E-10	2.96E-08	2.96E-08	0.03%
InH	1.82E-14	1.93E-12	1.93E-12	0.00%
H	6.01E-16	6.38E-14	6.38E-14	0.00%
SrH	2.63E-16	2.79E-14	2.79E-14	0.00%
BaH	1.51E-16	1.61E-14	1.61E-14	0.00%
SbH3	2.05E-22	2.18E-20	6.54E-20	0.00%
PbH	1.10E-25	1.17E-23	1.17E-23	0.00%
ZrH	4.12E-33	4.37E-31	4.37E-31	0.00%
SnH4	4.26E-45	4.52E-43	1.81E-42	0.00%
Total	4.54E-07	4.82E-05	9.47E-05	

Initial H (Mol/MTIHM)	0.023
% Volatilized	0.42%