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# Modeling Radionuclide Inventories in MSR Off-Gas Systems with Radiochemical Transport Analysis

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## ABSTRACT

Molten salt reactors (MSR) contain unique characteristics that may require enhancements to modeling tools to accurately predict phenomena. One characteristic that may be advantageous to leverage during normal operation is on-line processing of the circulating fuel salt, such as an off-gas system (OGS) to remove volatile fission products. Therefore, new modeling tools must be developed to integrate spatial resolution and chemistry effects into fuel depletion tools to be able to account for these non-core sources of radioactivity. Such types of radiochemical transport analysis tools were used to estimate the removal rates for 12 elements within a flow model of the Molten Salt Reactor Experiment (MSRE) by optimizing against legacy experimental data of the gas-borne (GB) percentages of 12 nuclides. The removal rates were used in a depletion model to calculate the FP inventory that enters the MSRE OGS. Calculations are in good agreement with the empirical GB percentages reported for the 12 nuclides, which validates the approach and verifies each tool's treatment of the radiochemical flow effects. The OGS inventory is discussed in terms of the largest nuclide contributors to activity, dose consequence, decay heat, and elemental composition. Finally, insights from the study allow recommendations to be made for future code development activities.

*Keywords*: molten salt reactors, mechanistic source term, off-gas system, radionuclides, species transport

## 1. INTRODUCTION

Liquid-fueled molten salt reactors (MSR) are a popular class of advanced (non-LWR) reactors currently under development. Many MSR designs have unique characteristics regarding radionuclide (RN) behavior that may require enhancement to modeling and simulation tools for use by regulators and designers as part of licensing applications. Specifically, one characteristic that may be advantageous during normal operation is on-line processing of the circulating fuel salt to improve various efficiencies. Developers may design the primary loop to include auxiliary systems, such as an off-gas system (OGS) to remove volatile fission products (FP) or a fuel processing system for breeding or chemistry control. In such cases, auxiliary systems can represent ex-core regions of the reactor where RNs may be removed from the fuel salt and stored for some period of time. Therefore, modeling such ex-core sources of RNs may be necessary to ensure adequate protection to the public [1]. This is required for licensing applications to model potential effluent source terms during normal operations or accident scenarios but is also advantageous for reactor design studies.

To support both the advanced reactor industry and U.S. Nuclear Regulatory Commission (NRC) in the pursuit of reactor design and licensing, the U.S. Department of Energy (DOE) Nuclear Energy Advanced Modeling and Simulation (NEAMS) program has established a mechanistic source term (MST) research

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project under the Multiphysics Applications technical area. MST analysis, or the realistic evaluation of RN transport from the source to the environment for specific transient scenarios, is central to the reactor licensing process and a focus of the NRC regarding their mission to provide reasonable assurance of adequate protection of public health, safety, and environment. The objective of the project is to coordinate the development of comprehensive advanced reactor MST mod/sim capabilities to support risk-informed design and licensing decisions. As such, an MST mod/sim development pathway was developed [2], which outlines the high-level objectives and near-term tasks necessary to achieve the project objectives. This work is one such recommended task to assist in the estimation of source terms in auxiliary systems of MSRs.

Two tools are demonstrated here for calculating radionuclide inventories in the OGS of the Molten Salt Reactor Experiment (MSRE). First, reduced order steady-state multi-region models based on Bateman equations are utilized to provide insights on radiochemical transport phenomena influencing the removal of RNs from the fuel salt to the gas phase in an ex-core region. Specifically, a lumped parameter approach is utilized to optimize scalar removal rate values for elements in the ex-core region to investigate how it influences the inventory of daughter RNs. The removal rates are optimized by comparing against experimental data for gas-borne (GB) percentages of several RNs measured in the pump bowl cover gas region of the MSRE. Second, a fuel depletion modeling tool is used to provide a first approximation of the FP inventory that likely entered the OGS of MSRE by applying the removal rates over a 2-year full-power burn-up with continuous chemical removal according to the reactor's unique flow model.

The OGS inventory results are discussed in units of elemental composition, activity, dose consequence, and decay energy, each motivating unique considerations in the design of the OGS. In addition to discussion of the results with respect to MST and design analyses, this work aims to further multiphysics capabilities in the tools developed under the NEAMS program. As such, recommendations are made for code development activities stemming from the results and experiences in this work.

## 2. ESTIMATING REMOVAL RATES

Fuel depletion calculations can be used to estimate RN inventories but rely on accurate estimates of removal rates that represent continuous on-line chemical removal. Such removal rates are estimated here by optimizing against historical MSRE data. The primary sources of experimental MSRE data providing insight into MSR chemistry effects are the radiochemically measured capsules of material that were extracted from the pump bowl of the reactor [3]. The pump bowl, located downstream of the core outlet and upstream of the heat exchanger, was where intentional chemical separations occurred by spraying the salt into a pool sparged with noble gases [3]. The cover gas region of the pump bowl was connected to the minimalistic off-gas system through a jumper line. Many samples were extracted from the pump bowl over the course of the reactor, including capsules filled with varying amounts of salt, gas, or mist.

A collection of samples during the $^{233}U$ operation mode of the reactor were made with double-walled freeze valve capsules designed to extract species from the cover gas of the pump bowl into the inner capsule through a nozzle. Because they believe mist likely contaminated the capsule, especially concentrating at the nozzle, they cut the capsule into multiple pieces to take separate measurements. The gross and net counts are reported [3], where the gross counts indicate the percentage of that radionuclide that they estimate to exist in the cover gas either as a gaseous species or as a mist. The net counts are the contributions from mist subtracted from the gross counts, therefore these "gas-borne" percentages represent the fraction of the RN that exists in the gas phase solely through volatilization of a precursor or itself, but not through aerosolization. These GB percentages are thus interpreted here as the vapor fractions of the respective RN in the cover gas of the pump bowl which are predominantly a function of the volatility of itself or its precursors. In this way, removal rates of several elements can be estimated by optimizing radiochemical transport models against these vapor fractions.

## 2.1. Radiochemical Transport Analysis

A modeling tool was previously designed to integrate depletion, chemical removal, and spatial flow effects into a reduced order model for simple and fast prediction of the steady-state inventory of fission products across regions of a MSR [4]. The model is especially useful in demonstrating the importance of radiochemical transport effects on FP inventories due to the wide variation in both yields and half-lives of FP precursors as well as chemistry, which may be unique to a specific region of the reactor. The source and loss terms for many FPs must be resolved by region to accurately compare calculation results to experimental measurements. Also unique to MSRE, the circulating salt did not enter the pump bowl with every pass, but rather only about 5% of the salt flow was diverted into the pump bowl, therefore the removal rate predicted with a spatially resolved model will be larger than that predicted if assuming the fuel salt is static and continuously being processed. For example, the mean GB percentage of $^{89}$Sr (5.7%) represents the amount of the nuclide that is in the gas phase because some (but likely not all) of its noble gas precursor (3.15-min $^{89}$Kr) transported from the core to the pump bowl before decaying. Because the half-life of the volatile precursor is similar in magnitude to the fuel salt residence time of the reactor, a portion of the noble gas FP is decaying in the salt before it can be extracted into the gas phase, thereby reducing the GB percentage of the $^{89}$Sr. Therefore, accurate estimates for elemental removal rates which are agnostic to the flow parameters of the reactor can only be solved for with a spatially resolved depletion tool. The flow model of the MSRE utilized here is the same as previously reported [4] with the fissile burn-up distribution as estimated by the operators: 93.5% of fissions from $^{233}$U, 2.2% from $^{235}$U, and 4.3% from $^{239}$Pu [3].

## 2.2. Method for Estimating Removal Rates

As mentioned, the GB percentages of several FPs were reported based on experimental measurements of gas samples during MSRE operation of $^{233}$U fuel, reproduced in Table I [3]. An optimization procedure is used here to estimate the removal rates of the FP element and/or its precursors which would result in the prediction of these GB percentages based on the net counts, which are meant to be interpreted as those excluding mists. The median values are utilized in the optimization procedure below because the skew of the data indicates mean values are disproportionately influenced by large outlier values. Additionally, it is clarified that the GB data represents multiple phenomena which might influence RN volatility such as vapor-liquid thermochemical equilibrium, physical solubility limits, and insoluble particle behavior. Therefore, this approach aims to lump the entirety of chemical effects which might volatilize nuclides in MSRs into one scalar removal rate that can simplify fuel depletion calculations. This study aims to show how limited legacy MSRE data can still be used to provide a first approximation of the RN inventory that may have entered the reactor's off-gas system as volatile species.

Initially, the noble gas elemental removal rate (assumed equivalent for Kr and Xe) was optimized separately against the data for each of the salt-seeking daughters in Table I, assuming only the noble gas precursor isobar is being removed in the pump bowl region. These initial four predictions for the noble gas removal rate differed considerably, which motivated an alternative optimization. First, the quality of the experimental data for $^{137}$Cs, $^{89}$Sr, and $^{140}$Ba appear sufficient, but the standard deviation for $^{91}$Y is larger than the corresponding mean or median, indicating a gas borne percentage close to zero with non-negligible sources of uncertainty. Therefore, $^{91}$Y data was not used to optimize the removal rate. Additionally, because of the relatively long half-life of $^{137}$Cs, it was postulated that some amount of this nuclide was removed as a result of vaporization of CsF in addition to the Xe precursor. Therefore, the noble gas removal rate was taken to be the average of values from individual optimizations for the $^{89}$Sr and $^{140}$Ba data, which were very close in value. Then, using this rate for $^{137}$Xe, the elemental removal rate for Cs was predicted by optimizing against $^{137}$Cs data. As expected, the alkali metal removal rate was considerably smaller than that of the noble gases. As such, including it in inventory calculations for the other three nuclides did not appreciably change the calculated gas borne percentages for $^{89}$Sr, $^{140}$Ba, and $^{91}$Y, i.e., the alkali metal precursors for these FPs are much shorter-lived and thus not as impacted by such a small removal rate in the pump bowl.

**Table I. Nuclide gas-borne percentage of the MSRE production rate (reproduced from [3])**

| Isotope | $t_{1/2}$ | Number | Range (%) | Median (%) | Mean ± σ (%) |
|---|---|---|---|---|---|
| **$^{137}$Cs** | 30.08 y | 9 | -1.6 – 91 | 23 | 25 ± 6 |
| **$^{89}$Sr** | 50.563 d | 11 | 0.06 – 15 | 3 | 5.7 ± 1.2 |
| **$^{140}$Ba** | 12.751 d | 11 | -0.004 – 0.18 | 0.027 | 0.056 ± 0.013 |
| **$^{91}$Y** | 58.51 d | 11 | -0.11 – 0.08 | 0.003 | 0.006 ± 0.010 |
| **$^{95}$Nb** | 34.991 d | 11 | -0.2 – 3.6 | 0.4 | 0.9 ± 0.2 |
| **$^{99}$Mo** | 65.924 h | 11 | -0.6 – 7.3 | 0.3 | 1.5 ± 0.5 |
| **$^{103}$Ru** | 39.247 d | 11 | 0.05 – 10 | 1.1 | 2.3 ± 0.7 |
| **$^{106}$Ru** | 371.8 d | 11 | -2 – 36 | 6 | 11 ± 3 |
| **$^{131}$I** | 8.0252 d | 11 | -0.1 – 2 | 0.2 | 0.5 ± 0.1 |

The removal rates for Nb, Mo, Tc, and Ru were estimated by optimizing against the experimental GB percentages of $^{95}$Nb, $^{99}$Mo, $^{103}$Ru, and $^{106}$Ru. Because $^{95}$Nb only has salt-seeking precursors, only the Nb chemical removal rate is optimized. This is held constant when optimizing the removal rate of Mo against the GB percentage for $^{99}$Mo. Then both the Nb and Mo removal rates are used to optimize the removal rates of Tc and Ru by comparing calculations against the GB percentage data of $^{103}$Ru and $^{106}$Ru simultaneously. It should be noted that the relatively large removal rate of Tc that is estimated is likely a result of unique chemistry behavior seen during $^{233}$U operation influencing noble metal transport on bubbles. Additionally, the steady-state assumption used here to represent the GB percentages may need to be revisited in future work as it is clear the longest-lived of the 12 nuclides analyzed here have the largest GB percentages.

The experimental data for two Te isotopes does indicate that the element is likely to exist in the cover gas region in the form of a mist to a small degree, but no conclusions can be made about its volatility as a gaseous species given the wide scatter of the data. It can be assumed that Te will enter the OGS because two isotopes were measured in the MSRE OGS jumper line with gamma spectroscopy [5]. The reactor's off-gas jumper line was an approximately 2 feet long, corrugated 1-inch inner diameter flexible tube connecting the fuel pump purge-gas exhaust at the pump bowl with the 4-inch pipe section of the off-gas line. This was the only portion of the reactor's OGS that was clearly visible from above without obstruction, therefore it is the only gamma spectroscopic data of the reactor's OGS. The operators noted that the third and final survey during the November 1969 shutdown represent the best estimates, reporting values for the average activity levels of: $^{95}$Nb, $^{99}$Mo, $^{103}$Ru, $^{106}$Ru, $^{125}$Sb, $^{126}$Sb, $^{127}$Sb, $^{129m}$Te, $^{131}$I, $^{132}$Te-I, $^{137}$Cs, and $^{140}$Ba.

In addition to Te, three isotopes of Sb were measured in the jumper line at significant activity levels, and they note that there was no indication that salt entered the OGS jumper line. Tin isotopes were not measured in the jumper line, therefore it is not assumed here to be volatile. Thus, removal rates for only Sb and Te are estimated here. Because estimates on the GB percentage of these elements are either not reported or contain a wide scatter, the gamma spectroscopic data of the OGS jumper line is qualitatively assessed in the following way to obtain removal rate estimates. First, for those nuclides where both GB percentage and OGS jumper line data are reported, the activities deposited on the jumper line are compared to their respective mean GB percentages. For six of the seven nuclides ($^{95}$Nb, $^{99}$Mo, $^{103}$Ru, $^{106}$Ru, $^{131}$I, $^{140}$Ba-La), it is found that between 3-13% of the total nuclide inventory in the cover gas region of the pump bowl can be

found deposited on the OGS jumper line. These deposition fractions were calculated using inventory values at the date of the November shutdown during the $^{233}$U operation of MSRE. The only nuclide that falls outside this range is $^{137}$Cs at around 0.2%. Comparing the shorter-lived $^{103}$Ru (~13%) with the longer-lived $^{106}$Ru-Rh (~3%) attempts to normalize out chemistry effects, indicating that the longer-lived isotopes of the same element may fall on the lower end of this range while the shorter-lived may fall on the higher end.

Nonetheless, comparing the 3-13% range with the total reactor inventory of the missing Sb and Te nuclides can provide an estimate of their GB percentages, and thus the Sb and Te elemental removal rates. The Sb removal rate was optimized by first estimating the GB percentage of 3.85-day $^{127}$Sb that would correspond to a deposition fraction value around 13%. This removal rate corresponds to a deposition fraction of 0.3% for 2.76-year $^{125}$Sb, which would follow the same behavior seen above for other longer-lived FPs. This Sb removal rate was then held constant in the Te removal rate optimization which similarly relied on estimating the GB percentage of 3.2-day $^{132}$Te that would correspond to a deposition fraction value around 13%.

Finally, the GB percentage of one iodine isotope is provided ($^{131}$I). Using the estimated removal rates for the precursor Sb and Te isobars, the removal rate of I was optimized against the reported median GB percentage. The same removal rate is also used for Br in this study. The estimated elemental removal rates discussed above are shown in Table II.

**Table II. Elemental removal rates for MSRE pump bowl region optimized from gas sample data**

| Element | Kr, Xe | Rb, Cs | Nb | Mo | Tc | Ru | Sb | Te | Br, I |
|---|---|---|---|---|---|---|---|---|---|
| **Rate ($s^{-1}$)** | 3.45E-3 | 6.08E-9 | 2.3E-8 | 2.19E-7 | 1.61E-3 | 3.29E-8 | 9.37E-8 | 1.22E-7 | 5E-8 |

No removal rate is assumed for the salt-seeking alkaline earth metals, lanthanides, or actinides, nor the fission product elements Rh, Pd, Ag, Cd, In, or Sn because of the lack of experimental data justifying their continuous on-line removal. Although it should be noted that some of these noble metals may adsorb on the surfaces of bubbles, allowing them to transport into the gas phase and OGS [6], further research is needed to clarify which elements exhibit this behavior and at what rate.

Finally, the removal rates predicted here are not to be interpreted necessarily as the rate at which these elements are removed from the circulating fuel salt, but rather just the rates at which these elements are extracted into the gas phase of the pump bowl, ultimately entering the off-gas system. The distinction is that the former accounts for the loss of these elements to other sources (such as depositing on structural materials throughout the reactor system) while the latter only accounts for the loss of elements to the cover gas of the pump bowl. Therefore, these rates are not necessarily representative of inventory losses from the circulating MSRE fuel salt but rather solely representative of the inventory gained in the OGS of the MSRE.

## 2.3. One-Region Removal Rate

The same approach as above was utilized with a one-region model with the objective of benchmarking against removal rate values which have been derived or used in other MSR fuel depletion studies. This was only completed for the continuous removal of the noble gas precursor of each $^{89}$Sr and $^{140}$Ba separately. The average of the two predicted removal rates was found to be 1.915E-04 $s^{-1}$, which is almost a factor of 20 smaller than the removal rate calculated in the multi-region model representative of the MSRE flow loop. This can be explained by the fact that only about 5% of MSRE fuel salt was sent to the pump bowl with every pass of the loop, therefore the removal rates that would be implemented only within the pump bowl region will undoubtedly be larger than rates applied continuously over the entire fuel salt inventory. As a benchmark, the one-region Xe removal rate constant for MSRE, MSDR, and MSBR were estimated recently through another method in a study aimed at investigating the impact of $^{135}$Xe removal on reactivity [7]. They report a removal rate value of 2.054E-04 $s^{-1}$ for MSRE, providing confidence in the approach

utilized here. Nonetheless, it is unclear if the use of one-region removal rates provides an accurate representation via continuous removal. An example of this reduced order error is that the shortest-lived FPs will likely never make it to the OGS and exit the salt, whereas the continuously processed one-region model will still remove these isotopes to some degree.

# 3. FUEL DEPLETION

Although the elemental removal rates estimated in the previous section are agnostic to the fissile source of as far as the differences in FP yields, there still may be indirect chemistry effects between different fuel cycles that influenced the GB data reported during the $^{233}U$ operation. For example, it has been shown that significantly different circulating void fractions were found between the $^{235}U$ and $^{233}U$ modes of operation which may have been caused by corrosion product behavior during salt redox potential transients during beryllium reductions which impacted multiphase flow [6]. Nonetheless, the removal rates estimated here may still provide a good approximation for the inventories in the MSRE OGS during any desired fuel cycle with the understanding that noble metals did behave differently in the $^{233}U$ runs compared with the $^{235}U$ runs. Because this is likely more a function of chemistry than a difference in fuel cycle [6], it should be noted that there is less confidence in the noble metal removal rates if being applied to other reactors.

Removal rates were applied continuously over 2 EFPY burn-up at 8 $MW_{th}$ using a MSRE fuel depletion model that has been previously reported [8], which utilizes MCNP for neutronics and ADDER for fuel depletion and chemical processing [9]. This tool is used in order to provide a benchmark for the NEAMS depletion tool Griffin which is currently being developed [10]. Novel multiphysics functionalities were recently demonstrated with Griffin, including its coupling with Thermochimica and MSTDB-TC for depletion-driven thermochemistry and its coupling with Pronghorn for spatially resolved depletion [10]. Because the spatially resolved capability currently only tracks a subset of nuclides and not the entire inventory, ADDER is utilized here to first develop a benchmark and inform Griffin development.

ADDER accounts for flow effects by completing loop transports between coarse depletion steps and removing elements or isotopes in specific regions at user-defined rates in units of fraction per second, accounting for the region's residence time. Because ADDER currently cannot track the removed inventories in a separate region, the OGS inventory is estimated by taking the difference between two depletion runs: a baseline with no chemical removal and an otherwise identical run with chemical removal of the 12 elements. Additionally, ADDER's MSR depletion results are representative of the inventory as it is entering the core, i.e., after completing a full loop transport; in the case of MSRE, this means the inventories are around 12 seconds downstream of the pump bowl outlet. Therefore, the results here should be interpreted as the OGS inventory after a cooling time of around 12 seconds.

The $^{233}U$ fuel composition used is based on the elemental composition of the carrier salt averaged across Runs 16-20 [11] and the same impurities as reported previously [8]. The fissile content is based on isotopic measurements from the end of Run 20 [11], which also includes Pu, as it was added to the reactor during operation. Based on these measurements, Pu consists of about 2% of the U content on a molar basis at shutdown, therefore this proportion of Pu was added at the isotopic composition reported. The depletion results are first validated by comparing with the empirical values used to optimize the removal rates, then the calculated GB percentages are interpreted as hypothetical inventories entering the OGS of MSRE.

## 3.1. Tool Verification and Approach Validation

Before discussing OGS inventory values, a preliminary verification and validation exercise is performed by (1) comparing ADDER calculations of the GB percentages for multiple Xe isotopes with those calculated by the steady-state model and (2) comparing ADDER calculations with the empirical values. Results from (1) are shown in Figure 1 and verify that each tool implements production terms, the flow model, and chemical processing in the ex-core region consistently. It is reiterated that these "GB percentages" are

calculated downstream of the pump bowl, therefore care must be taken in comparing these with GB percentages calculated elsewhere in the primary loop, especially for short-lived isotopes.

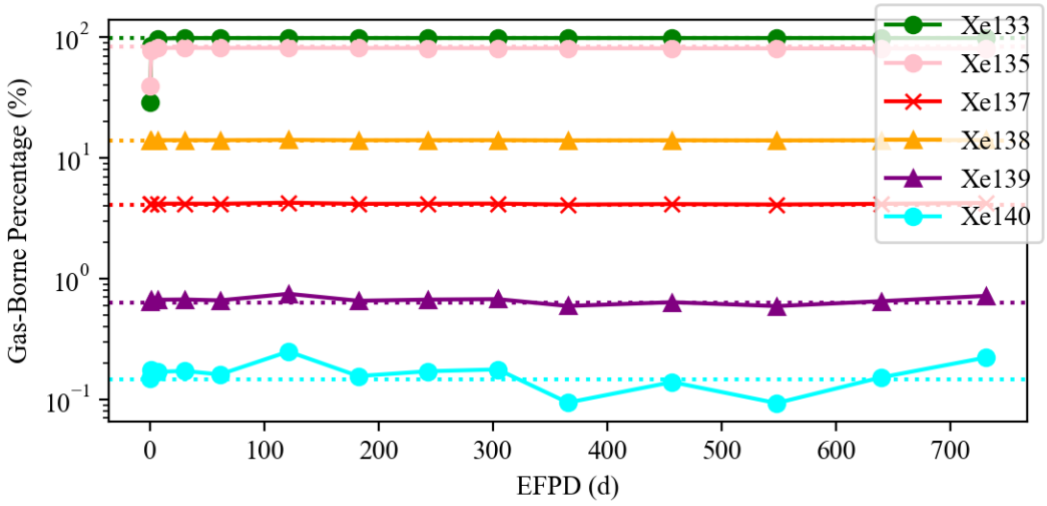


**Figure 1. Gas-borne percentages calculated over 2 EFPY of $^{233}$U MSRE operation using MCNP-ADDER depletion results (solid) or a Bateman equation-based steady-state model (dotted).**

Results from (2) are shown in Figure 2 in descending order of nuclide half-life and appear in good agreement with the empirically derived GB percentages for these isotopes, noting that the empirical values for $^{125}$Sb, $^{127}$Sb, and $^{132}$Te were estimated from gamma spectroscopic data as discussed in Section 2.2. The discrepancy seen for the longest-lived nuclides ($^{137}$Cs, $^{125}$Sb, $^{106}$Ru) is explained by the fact that the time-dependent depletion results have not yet reached equilibrium values, which are typically attained after ~5 half-lives. In this approach, removal rates were optimized from GB percentages assuming steady-state behavior, therefore using the removal rates will produce the expected GB percentages only as the RN approaches equilibrium. Future work may benefit by revisiting this steady-state assumption of the empirical GB percentage values, although MSRE operators did not report raw data, but rather only the distribution statistics, therefore the transient nature of the GB percentage data is unknown.

The two nuclides with the lowest GB percentages ($^{91}$Y, $^{140}$Ba) result in the other discrepancy seen, which can be explained by assumptions made regarding the quality of the data, as further discussed in Section 2.2. Because the standard deviations are much larger than the mean and median, the calculated results are still within the error bars. Overall, the approach utilized to continuously extract 12 different FP elements at various rates according to a unique flow model appears to estimate the GB percentages of 12 specific nuclides correctly. This is especially noteworthy given the large variations in half-life, FP yield, and chemistry behavior for not only the 12 nuclides themselves, but also their precursors. This helps validate the approach for estimating FP inventories in the MSRE OGS, which could be repeated for other MSRs provided the requisite experimental data representative of the reactor's chemical effects exists.

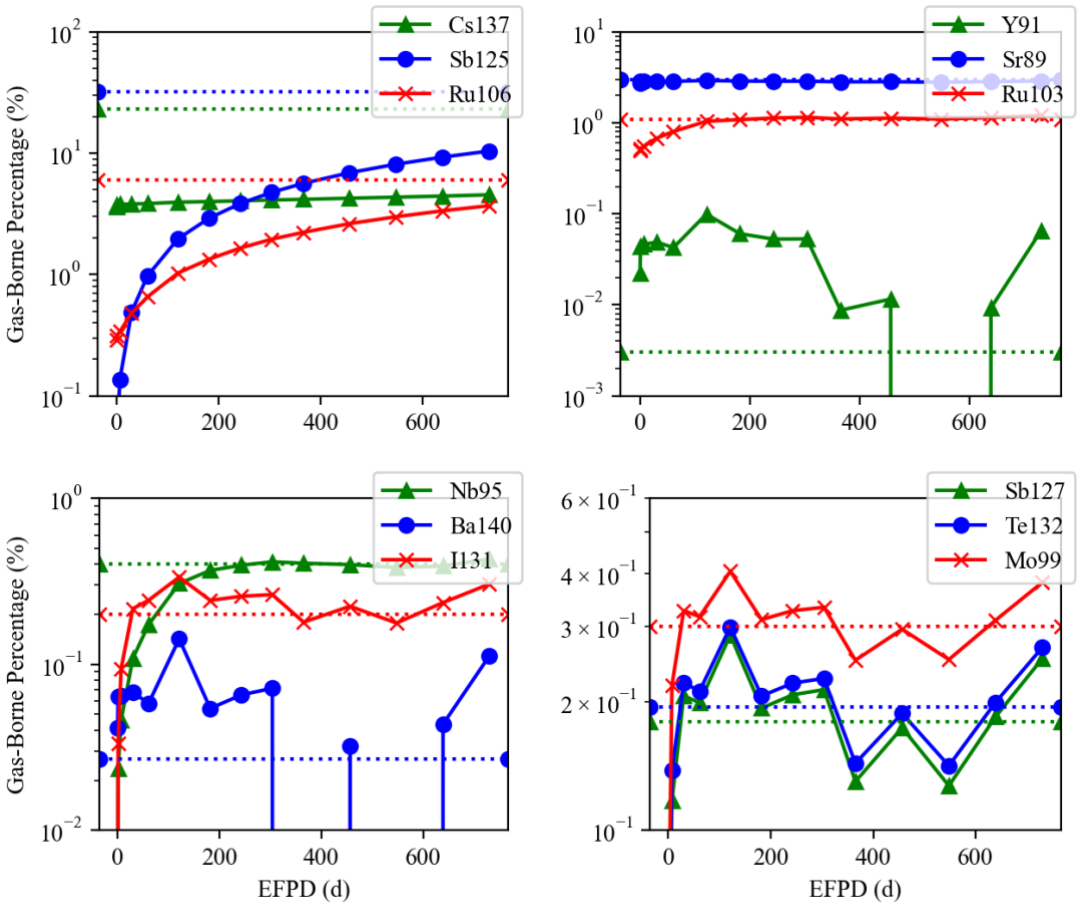


**Figure 2. Gas-borne percentages calculated over 2 EFPY of $^{233}$U MSRE operation using MCNP-ADDER depletion results (solid) compared against empirical gas-borne percentages (dotted).**

## 3.2. Radionuclide Inventories in the MSRE Off-Gas System

The OGS inventories are approximated by taking the difference between a baseline depletion run (i.e., no chemical removal) and a second depletion run with chemical removal using the rates estimated in Section 2.2. Because of small fluctuations in neutronics that might occur due to the processing of $^{135}$Xe and resulting influence on the fissile fraction, inventory differences may vary around a mean value over time. Therefore, reported here are the average values of the final eight timesteps (i.e., 6 months to 2 years). The results are reported using starting fuel based on the final $^{233}$U fuel isotopics, accounting for the many enrichment additions made. The top 10 nuclides are reported in Table III in terms of their percentage of the total inventory. And the results are displayed in terms of their contribution to activity, decay heat, total effective dose equivalent (TEDE), and elemental composition. The TEDE values are calculated from dose conversion factors (DCF) as tabulated in FGR 11 and 12 [12, 13]. Decay heat is calculated using each nuclide's total energy released per decay in eV which are tabulated in ENDF/B-VIII.0 along with decay constants.

Not surprisingly, the FP noble gases comprise many of the largest contributors in all four categories, including over 50% of the total decay heat contribution and elemental composition, owed to the large removal rate estimated and implemented for Kr and Xe. As a result, several Rb and Cs isotopes are also significant contributors, including nearly 40% of the total decay heat, motivating the careful design of OGS stages that can scrub these alkali metals from the gas stream under high heat loads. It can also be seen that

the FP noble gases account for over 1/3rd of the TEDE consequence if released to the environment without additional hold-up. Fortunately, nearly all FP noble gases have half-lives on the scale of hours to days, therefore proper design of capture or hold-up stages can drastically reduce the activity and dose consequence, although considerations for their decay heat should be taken when designing such stages. Considerations should also be taken for dose and radiochemical effects of Tc and Ru transporting in the OGS as they appear to be significant in all categories, including nearly 25% of the TEDE consequence. This is also owed to the large removal rate used for Tc, which should be further investigated in future experimental work, especially as a function of multiphase flow dynamics. And it is worth noting that despite the low removal rates for iodine and its precursors, $^{131}$I is still one of the top contributors to dose consequence. Therefore, further experimental work to characterize the volatility of I, Te, and Sb would be beneficial to ensure the removal rates are not much larger.

**Table III. Largest OGS contributors for $^{233}$U MSRE (average % of total over 0.5 - 2 EFPY)**

| Nuclide | Activity | Nuclide | Decay Heat | Nuclide | TEDE | Element | Molar Composition |
|---|---|---|---|---|---|---|---|
| **$^{133}$Xe** | 22.77% | $^{88}$Rb | 28.34% | $^{88}$Kr | 22.68% | Xe | 43.27% |
| $^{135}$Xe | 12.66% | $^{88}$Kr | 24.11% | $^{106}$Ru | 20.28% | Cs | 17.19% |
| $^{88}$Rb | 12.46% | $^{87}$Kr | 12.02% | $^{88}$Rb | 9.24% | Kr | 10.54% |
| $^{88}$Kr | 12.45% | **$^{138}$Cs** | 7.99% | $^{89}$Sr | 7.26% | Tc | 8.94% |
| $^{99m}$Tc | 11.22% | **$^{135}$Xe** | 6.00% | **$^{138}$Cs** | 6.20% | Sr | 5.99% |
| $^{87}$Kr | 6.79% | **$^{138}$Xe** | 4.02% | $^{87}$Kr | 5.00% | Rb | 5.47% |
| $^{85m}$Kr | 5.90% | **$^{133}$Xe** | 3.48% | **$^{134}$Cs** | 4.41% | Mo | 5.18% |
| $^{138}$Cs | 2.66% | **$^{85m}$Kr** | 2.03% | **$^{138}$Xe** | 2.72% | Ba | 1.29% |
| $^{138}$Xe | 2.64% | **$^{89}$Kr** | 1.82% | **$^{135}$Xe** | 2.69% | Ru | 1.04% |
| $^{83m}$Kr | 2.08% | **$^{89}$Rb** | 1.78% | **$^{131}$I** | 1.81% | Te | 0.47% |

## 4. RECOMMENDATIONS FOR CODE DEVELOPMENT

Important outcomes of this work are the insights and recommendations for future code development activities to improve MSR species tracking capabilities in NEAMS modeling tools. A multiscale and multiphysics depletion model representative of the MSRE with chemical processing is currently being developed using Griffin, Pronghorn, and Thermochimica which can soon be used to estimate the removal rates not only as in Section 2.2, but to much higher mesh discretization and spatial fidelity if desired [10]. The improved NEAMS framework will enable state-of-the-art species tracking and RN inventory accounting for MST analyses. The multiscale functionality will allow for certain nuclides to be tracked explicitly in space with high resolution, and while others are lumped and solved with reduced order resolution for increased computational performance. Subsequent models using continuous or batch extraction of nuclides from the NEAMS depletion suite results should be tested and verified against results such as those presented here and the original experimental data. The ability to track the inventory in an ex-loop region is necessary for modeling auxiliary systems and is already being developed in Griffin. Once an inventory is predicted in an ex-loop region, a tool to track RN inventories throughout multiple stages of the OGS including reactions with processing components (i.e., only decay and chemical processing across different stages) will be needed. This type of multi-stage ex-core fuel depletion modeling can be used to show how chemical processing parameters (e.g., elemental removal and decay time) can influence RN inventories over time, such as during transients, without needing to account for the effects of reactor physics. Each of the functionalities discussed above serve different purposes in estimating RN inventories in a MSR OGS, and the goal will be to benchmark future NEAMS tools against the preliminary results reported here.

## 5. CONCLUSIONS

Elemental removal rates that can be used in depletion calculations with lumped parameter system level species transport were estimated from MSRE experimental data. The data used to optimize the removal rates consisted of empirical gas-borne percentages in the pump bowl. The elemental removal rates were used in a fuel depletion model to estimate the FP inventory that entered the MSRE OGS during $^{233}U$ operation. Calculations are in good agreement with the empirical data reported for 12 nuclides, validating the approach and each tool's treatment of the flow model. The OGS FP inventory is discussed in terms of the largest nuclide contributors to activity, dose consequence, decay heat, and elemental composition.

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