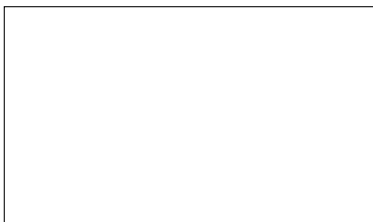


Graphical Abstract

Dynamic Mass Accountancy Modeling of a Molten Salt Reactor Using Equilibrium Thermodynamics

Max Poschmann, Markus H.A. Piro, M. Scott Greenwood



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Highlights

Dynamic Mass Accountancy Modeling of a Molten Salt Reactor Using Equilibrium Thermodynamics

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- Coupling of equilibrium thermodynamics library Thermochemica with dynamic systems modeling tool TRANSFORM
- Mass accountancy in a model of a molten salt reactor

Dynamic Mass Accountancy Modeling of a Molten Salt Reactor Using Equilibrium Thermodynamics

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Abstract

A mechanistic-based mass accountancy model in the context of molten salt reactors was implemented in the dynamic systems modeling software library TRANSFORM by way of coupling with the equilibrium thermodynamics code Thermochemica. Liquid-fueled molten salt reactors present new challenges for mass accountancy because of the dissolution of fuel and evolved fission products, which may be soluble in the salt, off-gas, or precipitate. Two cases of mass loss from the molten salt were addressed: off-gassing and precipitation. The software implementation was tested through a series of increasingly complex demonstration problems, culminating in a model of the primary fuel and primary coolant loops of the molten salt demonstration reactor. Analysis shows that negligible mass was lost from the salt under normal operating conditions, but an overheating event caused by partial loss of fuel loop cooling resulted in release of measurable amounts of uranium (among other elements) via off-gassing. The tools developed here are primarily aimed at capability development but are readily available for use in further modeling of molten salt reactor concepts. These tools have not yet

been validated, and future experimental work to perform this validation is recommended.

Keywords: Molten salt reactor, Gibbs energy minimization, system model, TRANSFORM, Thermochemica, Mass accountancy

1. Introduction

Mass accountancy in nuclear reactors is a fundamental component of the safety and security analysis required for licensing and safeguarding. Although mass accountancy in solid-fueled reactors is well understood in many cases, liquid-fueled reactor designs—including many molten salt reactor (MSR) concepts—pose new challenges [1]. In solid-fueled reactors, the fission and activation products are largely contained by the fuel and the surrounding cladding. In liquid-fueled MSRs, the fissile material is dissolved in a salt that flows throughout the primary fuel loop and interacts with numerous components, possibly altering the salt chemistry and certainly creating disparate thermodynamic conditions within the primary fuel loop. Moreover, fission products are created and transported in the core, which also alters the salt chemistry. In addition to obvious corrosion concerns, systems that model mass accountancy in liquid-fueled MSRs must be able to accommodate complex chemistry over a wide range of compositions and temperatures. Because tabulated chemical data representing this information at sufficient resolution would be prohibitively large, a Gibbs energy minimization (GEM) [2] approach was proposed [3].

To incorporate GEM into a mass accountancy model, two pieces are necessary: a thermodynamic database representing the system of interest and

a software library capable of performing thermodynamic calculations using that database. The Molten Salt Thermodynamic Database (MSTDB) [4] was used in this work. The most recent release of the MSTDB includes 14 elements (Pu, U, Th, Nd, Ce, La, Cs, Rb, Ca, K, Na, F, Be, and Li); 158 stoichiometric phases; and 25 solution phases that include a liquid solution of all 14 elements represented by the modified quasi-chemical model in the quadruplet approximation (MQMQA) [5, 6, 7, 8, 9], which is the state-of-the-art framework for molten salt phase models. A total of 46 pseudo-binary and 27 pseudo-ternary systems have been assessed in this database. The database is at an early stage of development and is expected to continue to mature in the coming years. To the authors' knowledge, calculations involving the MQMQA can be performed by only two thermodynamics libraries at this time: FactSage [10] and Thermochemica [11]. Of these, only the latter can be easily coupled to other software for the purposes of multiphysics simulations [12, 13, 14, 15, 16, 17].

The Transient Simulation Framework of Reconfigurable Models (TRANSFORM) is a Modelica-based, system-modeling library developed at Oak Ridge National Laboratory [18]. TRANSFORM enables rapid configuration and modeling of energy systems, including nuclear power reactors [1]. Because TRANSFORM has been used to model MSRs [1, 3], numerous relevant components and demonstration configurations are already available. However, TRANSFORM lacks a GEM solver, which has been identified as a gap in capability limiting its application for mass accountancy in MSRs [3].

To combine these capabilities, Modelica functions have been developed and incorporated into TRANSFORM to set up, run, and retrieve information

from Thermochemica calculations. Models of reactor components that make use of these functions, such as off-gas removal systems and solid precipitate filters, have been added as well. These classes are described in Section 2. The aforementioned reactor component models have been added to demonstration problems based on MSR subsystems of increasing complexity from a simple salt pot with an off-gas removal system to a model of the primary fuel and primary coolant loops of the Molten Salt Demonstration Reactor (MSDR). The MSTDB is used throughout these examples, which are discussed in Section 3. Opportunities for future work using this coupled code system are discussed in Section 4, and conclusions drawn from these demonstrations are presented in Section 5.

2. Incorporation of Thermochemica into Modelica Models

Two phenomena through which fissile materials might leave the molten salt solution were identified: off-gassing and precipitation. Corresponding component models that invoke Thermochemica were created to determine the amounts of phases present and the compositions of those phases. The off-gas removal component may be connected to any fluid volume component and determines the partial pressures of all gaseous species given the average composition, temperature, and pressure of the volume. Optionally, a second volume (i.e., head space) can be connected to the off-gas removal component to which these gas species are conveyed at a rate depending on the pressure difference between the first volume and the head space, as well as the specified efficiency of the off-gas removal component. The precipitate filter behaves similarly, except that it may be connected between any two

volumes or pipe elements. It removes mass corresponding to the amounts and compositions of solid phases predicted to be stable at equilibrium by Thermochemica, multiplied by the mass flow rate and component efficiency. These components can be used a number of times within a system model. Optionally, both employ the Thermochemica re-initialization algorithm to improve computational performance [19].

The current version of MSTDB permits only exact stoichiometric ratios of cations and anions to exist in the liquid molten salt phase. This is an unfortunate limitation because both leaching of metals from reactor components into the salt and the creation of fission products could lead to an excess of cations relative to anions in the salt. However, this problem is ameliorated somewhat by the presence of other liquid phases containing solely cation species (for example, pure K liquid). However, the current version of the MSTDB does not include a F_2 gas species or other species containing an excess of F (the only anion in the MSTDB) relative to cations. This means that the database cannot produce any result for a system with an abundance of F (e.g., 1 mole Li + 2 moles F). This has a negative effect on the stability of GEM calculations near or at stoichiometric cation-to-anion ratios. To improve this stability, the MSTDB used for the following calculations was slightly modified such that vacancies were permitted on the cation sublattice of the liquid molten salt phase. These cation vacancies are energetically unfavorable and usually present at concentrations of less than 10^{-20} , but they have a considerable positive impact on Thermochemica's performance.

Because of the absence of many fission products from the version of the MSTDB used in this work, using unmodified reactor kinetics data in

TRANSFORM in conjunction with Thermochemica would result in unrealistic changes to the salt chemistry during fuel burnup. Analysis of fission products created by uranium fission using ORIGEN-S [20] indicate that this reaction is slightly reduced. However, if only those fission products included in the MSTDB are considered, the fission reaction becomes strongly oxidizing. For the sake of simplicity, in the following demonstration problems the fission of one mole of U produces one mole each of Li, Na, K, and Cs for the purposes of chemistry calculations in Thermochemica only. Since the primary oxidation state of U is 4+ and each of the four products are in the 1+ state, this results in no net oxidation or reduction caused by fission. This approximation does not otherwise affect any of the heat transfer or reactor kinetics calculations in TRANSFORM.

3. Demonstration Problems

System models that incorporate the off-gas removal and precipitate filter components were built up from minimum viable systems to detailed MSR models. The configurations of these demonstration problems are summarized in Table 1. All demonstration problems were executed on a Linux workstation.

3.1. Salt Pot

For the off-gas removal system, the most basic example (shown in Figure 1) was a salt vessel (pot) with controlled heat input connected to a head space through the off-gas removal component. In this model and the following models, red lines indicate heat transfer, green lines indicate mass transfer, and blue lines indicate both heat and mass transfer between connected

Table 1: Summary of demonstration problem configurations. All species fractions are in mole percent and represent initial concentrations.

	Salt pot	Precipitate filter	Simple loop	MSDR	MSDR LOCA
Offgas enabled	✓		✓	✓	✓
Precipitate filter enabled		✓	✓	✓	✓
Point-kinetics feedback enabled					✓
LiF fraction	41.85%	41.85%	41.89%	41.89%	41.89%
NaF fraction	10.35%	10.35%	10.36%	10.36%	10.36%
KF fraction	37.80%	37.80%	37.84%	37.84%	37.84%
Cs fraction	10.00%	-	-	-	-
UF ₃ fraction	-	0.10%	4.50%	4.50%	4.50%
UF ₄ fraction	-	9.90%	4.50%	4.50%	4.50%
PuF ₃ fraction	-	1.00%	0.90%	0.90%	0.90%
Simulation time (s)	20,000	10,000	10,000	3.154×10^7	100,000
Run time (s)	15	9	243	949	997

components. Unconnected blocks represent various inputs to the system. This model system was based on the salt-to-gas transfer model presented previously by Greenwood and McMurray [3], with the partial pressure table replaced by Thermochemica. The off-gas removal component was used to monitor the composition of the gas volatilizing from the salt pot. The salt pot was initially filled with 41.85% LiF, 10.35% NaF, 37.80% KF, and 10.00% Cs (all molar fractions). The system was modeled for 20,000 s, and two 5,000 s long heat inputs were supplied (at 500 s and 10,500 s) to the salt pot to increase the temperature from the initial value of 500°C to 1,000°C and then to 1,500°C. Then, the change in the amount of volatilized elements was observed.

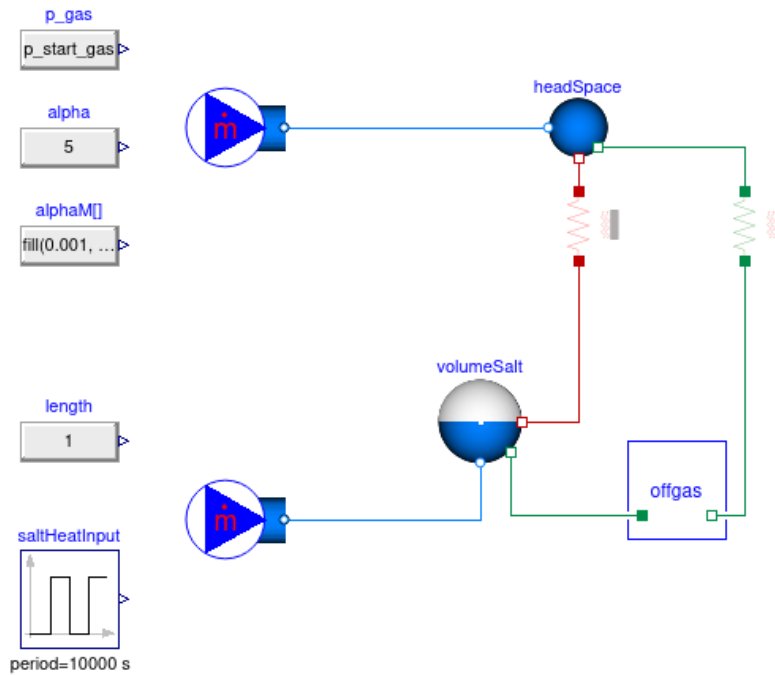


Figure 1: Salt pot example system using the off-gas removal component (“offgas”).

The predicted salt volume, temperature, system pressure, and the partial pressures of the volatilized elements are shown in Figure 2. Note that F_2 and CsF species do not exist in the gas phase in the current version of the MSTDB. Therefore, these results may differ significantly from reality, as well as from future calculations performed with an updated and more comprehensive database. Initially (i.e., near-normal operating conditions), the partial pressure of Cs was highest. After heat input was applied and the temperature began to rise, the amounts of other volatile elements (particularly K) increased rapidly. Competition with these volatilized elements caused the fraction of Cs in the gas (and thus the Cs partial pressure) to drop. This reveals that although Cs is the first fission product to volatilize at nominal reactor operating conditions, an increase in the temperature above $750^\circ C$ does not increase the amount of Cs released. Because F is the only anion present in the current molten salt model and the initial composition had an excess of cations, very little F volatilized until a significant portion of the salt boiled at above $1,000^\circ C$.

3.2. Precipitate Filter

The minimum viable system utilizing the precipitate filter component is shown in Figure 3. This system was a flowing salt loop consisting of a pump, a vessel, and the precipitate removal component. This example system was modeled for 10,000 s. The initial temperature was set to $550^\circ C$, and a 5,000 s long heat output from the salt vessel beginning at 500 s reduced the temperature to $500^\circ C$. The salt volume was initially filled with 41.85% LiF, 10.35% NaF, 37.80% KF, 0.10% UF_3 , 9.90% UF_4 , and 1.00% PuF_3 (all molar fractions). The temperature history and precipitate mass removed

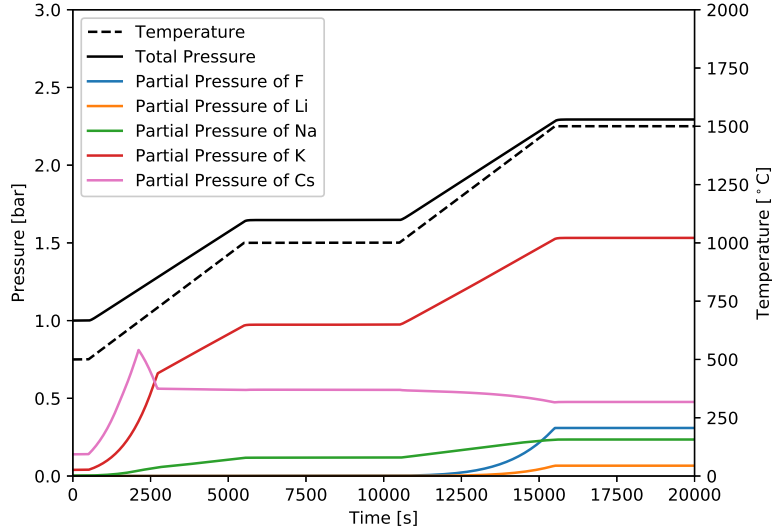


Figure 2: The salt pot temperature and pressure and the predicted off-gas partial pressures for the salt pot example system.

are plotted in Figure 4. At the initial temperature, no solid precipitate is predicted to form, but as the system cools below 525°C , solids (chiefly KF) are predicted to precipitate out of the molten salt. This indicates that the addition of uranium and plutonium species to the salt increase the melting temperature from the eutectic FLiNaK value of 454°C [21] to approximately 510°C , which is reasonable for such large additions of high-melting point species. Also, this temperature is still under the acceptable value of 550°C recommended by Grimes *et al.* to provide an appropriate margin of safety below the minimum operating temperature [22]. Note that the masses in this example are arbitrary for demonstration purposes and do not reflect a real MSR reactor design.

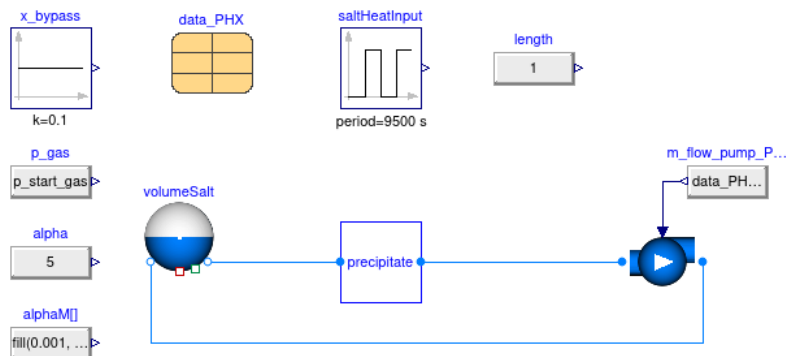


Figure 3: Precipitate filter example system using the precipitate filter component (“precipitate”).

3.3. Simple Loop

After ensuring that the new components functioned as intended, the authors simulated increasingly realistic scenarios, including burnup of fissile isotopes and generation of fission products through TRANSFORM’s reactor kinetics models. The first of these was a simple salt loop, as shown in Figure 5, featuring an inlet, outlet, two pipes, one larger volume element, and the two new Thermochemica-driven components. This model is a slightly enhanced version of the base model; periodic boundary conditions and additional loop elements were presented in a previous report [3]. The initial composition of the salt for this demonstration problem was 41.89% LiF, 10.36% NaF, 37.84% KF, 4.50% UF₃, 4.50% UF₄, and 0.90% PuF₃ (all molar fractions). The salt in the volume element was initially at 550°C, but input salt at the inlet was held at 350°C, resulting in the predicted salt temperature decreasing to 453°C over the course of the 10,000 s simulation. Figure 6 demonstrates that at these temperatures, no meaningful amount of any element volatilizes. On the other hand, as the temperature drops, a solid

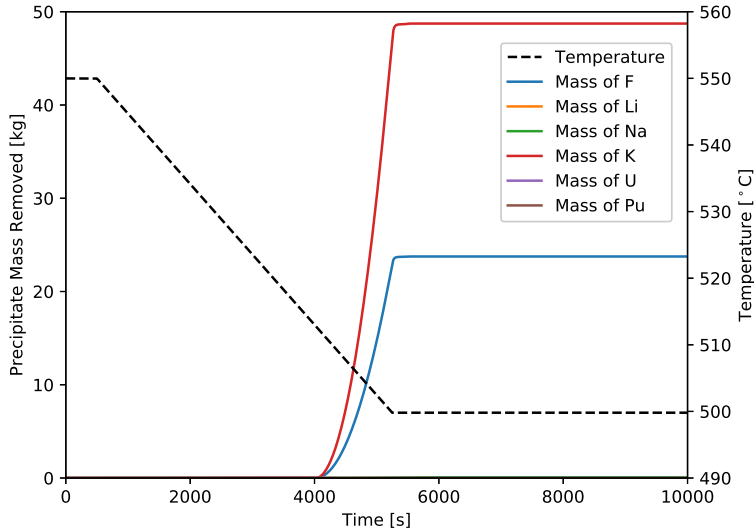


Figure 4: The salt temperature and the predicted precipitate mass removed from the precipitate filter loop example system. Only removal of KF is predicted in this scenario.

KF phase is predicted to precipitate and is removed by the precipitate filter, as seen in Figure 7.

3.4. MSDR

The most complex demonstration system is a model of the primary fuel and coolant loops of the MSDR, which was presented by Greenwood *et al.* [1]. The new Thermochemica-driven mass accountancy components were attached to the volume element at the top of the loop (downstream from the reactor core). This demonstration system model is shown in Figure 8. Again, the initial composition of the salt was 41.89% LiF, 10.36% NaF, 37.84% KF, 4.50% UF₃, 4.50% UF₄, and 0.90% PuF₃ (all molar fractions). The duration of the simulation was one year; the new components were switched on after 1,000 s, and no significant amounts of any element were collected by either

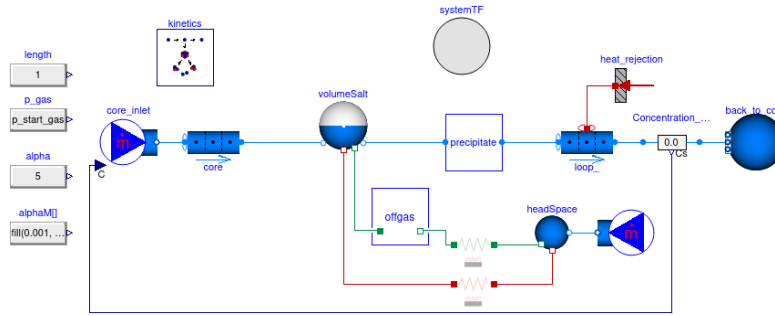


Figure 5: Simple loop demonstration configuration featuring combination of Thermochemical-driven mass accountancy components and reactor kinetics calculations.

the off-gas removal system or the precipitate filter under normal operating conditions. Collected masses of all elements were less than 0.1 g out of the total 111,880 kg total mass of the salt, and they consisted almost entirely of KF. This result is likely to be significantly different given a more complete thermodynamic database. Specifically, it is expected that noble gases such as Kr and Xe would likely dominate the off-gas that is removed.

3.5. MSDR LOCA

One of the key features of dynamic systems modeling of nuclear reactor designs is the capacity to simulate accident scenarios representing realistic component failures. To demonstrate this capacity, the MSDR model described above and shown in Figure 8 was modified such that the primary coolant loop pump flow rate was reduced to 5% of its initial value over the course of 25,000 s, beginning at 50,000 s into the simulation, and the simulation continued for another 25,000 s. For this simulation, the reactor power was determined using feedback from TRANSFORM's point-kinetics model [1, 23], whereas in the previous demonstration simulations, the reactor

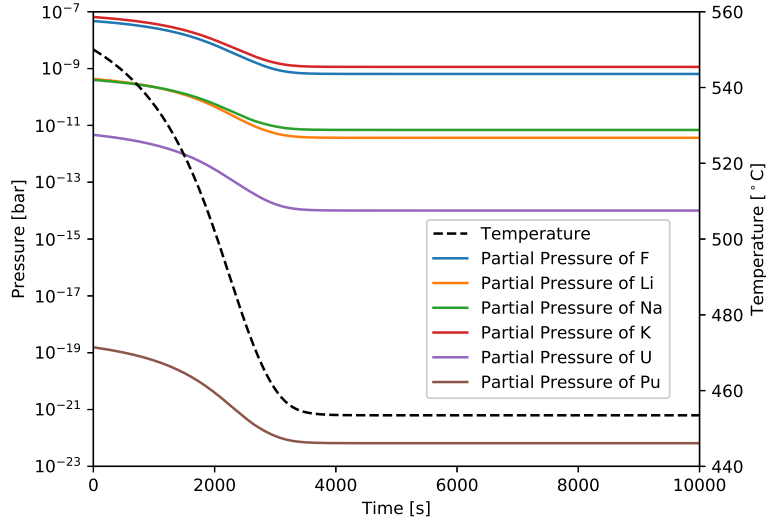


Figure 6: Temperature of salt volume element during the simple salt loop demonstration, as well as the (negligible) partial pressures of volatilized elements.

power was held constant. The results using the point-kinetics model showed a significant increase in the run time of the simulation. The reduction in flow rate caused less cooling of the primary fuel loop at the heat exchanger, thereby reducing the power output of the reactor. This represents a possible loss-of-coolant accident (LOCA) scenario. Because of the inherent safety features of molten salt reactors, the heat output falls as the pump power is reduced, resulting in a decrease of the primary fuel loop temperature from 722°C to 706°C. This slightly decreases the predicted partial pressures of all elements in the gas, as shown in Figure 9. During this accident scenario, no significant release of material was predicted by the model.

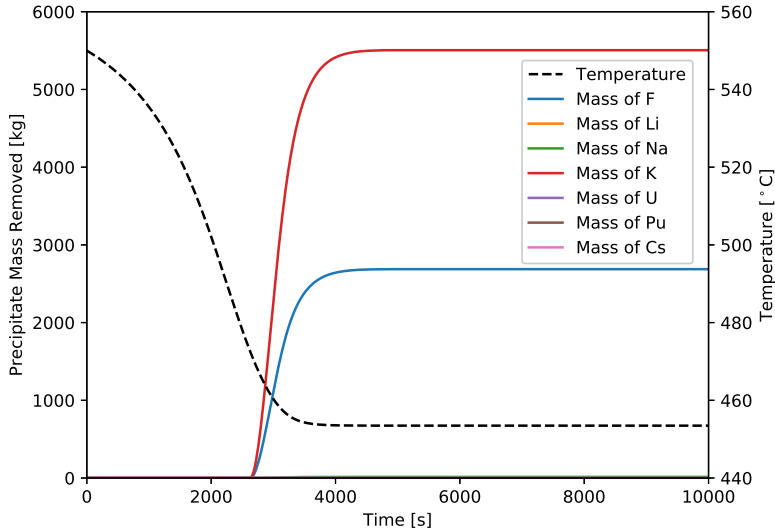


Figure 7: Amounts of elements removed by the solid precipitate filter in the simple salt loop demonstration.

4. Future Work

The flexibility and reusability of TRANSFORM components make it easy to use Thermochemica-driven mass accountancy in future simulations of MSRs. These simulations will include new reactor concepts as they are developed, as well as more complete models of existing reactor concepts (e.g., models including secondary coolant loops and beyond). There also remains considerable room to improve the component models presented here. For example, a more complex five-stage off-gas trap model based on the decay of Xe isotopes into Cs has been proposed [3], but it was not implemented here because Xe is not present in the current version of the MSTDB. New but related component models are likely needed as well. Noble metal plate-out on heat exchangers is an area of concern for MSR design because it may

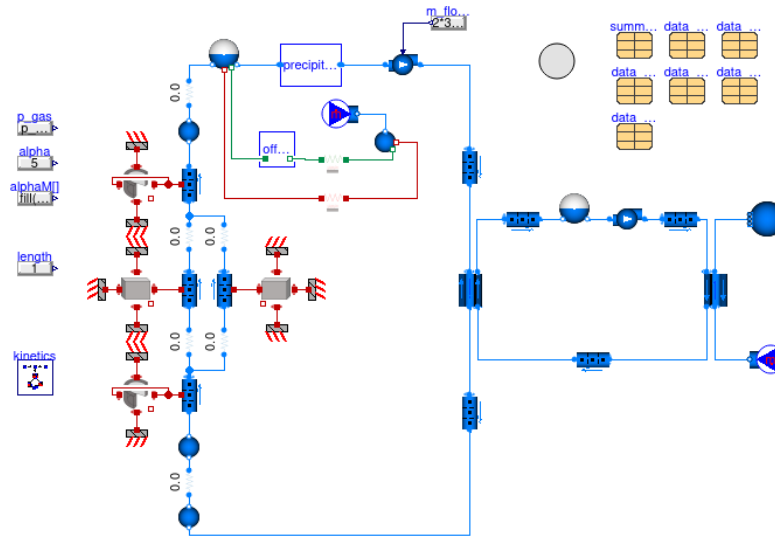


Figure 8: MSDR primary fuel loop and primary coolant loop demonstration configuration. New components “offgas” and “precipitate” were inserted downstream from the reactor core.

result in damage or reduced cooling effectiveness [24]. However, plate-out is strongly dependent on surface energy terms, which are not part of the MSTDB or other thermodynamic databases. A TRANSFORM component capable of predicting plate-out accurately would have to combine Gibbs energies of metastable phases predicted by Thermochemica with surface energies from another source. Thus, this remains a subject for future endeavors.

Other improvements to the models presented will become possible as the range of available thermodynamic data grows. More accurate coupling between reactor kinetics and chemistry requires a wider range of fission products to be present in the MSTDB. Mass accountancy for some isotopes of concern (such as radioactive isotopes of Xe, Kr, Br, and I) cannot be performed with the presently available data. It is not uncommon for Xe and

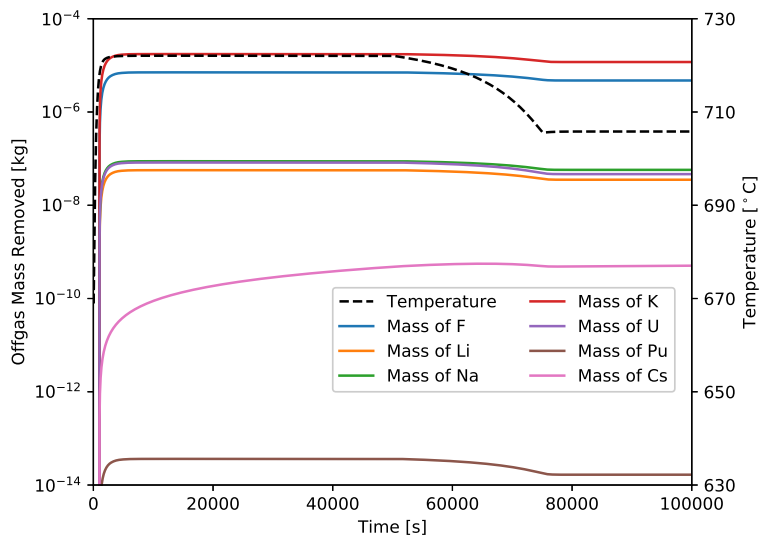


Figure 9: Amounts of elements removed by the off-gas removal system in the MSDR; loss of cooling started at 50,000 s.

Kr to be excluded from a thermodynamic database since they are generally chemical inert [25]; however, it may be useful to include Xe and Kr in future developments of the database to inform other parts of TRANSFORM. Iodine is certainly an important fission product to consider because it is chemical volatile and radioactively short lived, which is of general concern in the event of an accident [26]. Other fission products that may be worth adding to the database include the noble metals (e.g., Mo, Ru, Tc, Rh, Pd) and several elements known to form stable oxides (e.g., Ce, Nd, and Y), which may be important in accident scenarios in which the salt is in contact with air. At this time, it is unclear how significant certain fission products might be in the context of molten salts—prioritization efforts would help guide future studies to expand the database. As a database grows, the computational expense of

adding new elements grows geometrically because interactions between the new element and combinations of the elements already in the database must be determined either from experimental or first-principles data.

Validation of these models is an important outstanding task. Experiments performed on simple systems similar to those modeled here would provide valuable inputs for validation, especially if a more complete thermodynamic database were available to update the model predictions. In particular, experimental validation for the salt pot configuration would provide significant feedback while requiring only a relatively simple experimental apparatus.

5. Conclusions

Two new mass-accountancy components for the dynamic systems modeling library TRANSFORM were implemented, both employing the equilibrium thermodynamics GEM library Thermochemica to obtain the amounts and compositions of the phases present. These components enable physics-based mass accountancy over a broad range of temperatures, pressures, and compositions. The new capabilities for MSRs were demonstrated through simulations of nominal and accident scenarios for the MSDR. These components and those derived from them and their underlying functions could be used for rapid development and safety analyses of evolving nuclear reactor designs, in particular for MSRs. Because both TRANSFORM¹ and Thermochemica²—including the functions required to interface between the two—are publicly available on GitHub, the developments presented here en-

¹github.com/ORNL-Modelica/TRANSFORM-Library

²github.com/ORNL-CEES/thermochemica

able any interested parties to study mass accountancy in MSRs.

References

- [1] M. S. Greenwood, B. R. Betzler, A. L. Qualls, J. Yoo, C. Rabiti, Demonstration of the advanced dynamic system modeling tool TRANSFORM in a molten salt reactor application via a model of the molten salt demonstration reactor, *Nuclear Technology* 206 (3) (2020) 478–504.
- [2] W. B. White, S. M. Johnson, G. B. Dantzig, Chemical equilibrium in complex mixtures, *The Journal of Chemical Physics* 28 (5) (1958) 751–755.
- [3] M. S. Greenwood, J. W. McMurray, Prototype demonstration of an integration of a gibbs energy minimizer with TRANSFORM for molten salt reactor mass accountancy studies, Tech. rep., Oak Ridge National Laboratory, Oak Ridge, TN (United States) (2020).
- [4] T. M. Besmann, J. Ard, S. Utlak, J. W. McMurray, R. A. Lefebvre, Status of the salt thermochemical database, Tech. Rep. ORNL/SPR-2019/1208, Oak Ridge National Laboratory, Oak Ridge, TN (United States) (2019).
- [5] A. Pelton, S. Degterov, G. Eriksson, C. Robelin, Y. Dessureault, The modified quasichemical model I – binary solutions, *Metallurgical and Materials Transactions B* 31B (2000) 651–659.
- [6] A. Pelton, P. Chartrand, The modified quasichemical model II – multi-

- component solutions, *Metallurgical and Materials Transactions A* 32A (2001) 1355–1360.
- [7] P. Chartrand, A. Pelton, The modified quasichemical model III – two sublattices, *Metallurgical and Materials Transactions A* 32 (2001) 1397–1407.
- [8] A. Pelton, P. Chartrand, G. Eriksson, The modified quasichemical model IV – two-sublattice quadruplet approximation, *Metallurgical and Materials Transactions A* 32 (2001) 1409–1416.
- [9] G. Lambotte, P. Chartrand, Thermodynamic optimization of the (Na₂O + SiO₂ + NaF + SiF₄) reciprocal system using the modified quasichemical model in the quadruplet approximation, *Journal of Chemical Thermodynamics* 43 (2011) 1678–1699.
- [10] C. Bale, P. Chartrand, S. Degterov, G. Eriksson, K. Hack, R. Mahfoud, J. Melançon, A. Pelton, S. Peterson, FactSage thermochemical software and databases, *CALPHAD* 26 (2) (2002).
- [11] M. Piro, S. Simunovic, T. Besmann, B. Lewis, W. Thompson, The thermochemistry library THERMOCHIMICA, *Computational Materials Science* 67 (2013) 266–272.
- [12] M. Piro, J. Banfield, K. Clarno, S. Simunovic, T. Besmann, B. Lewis, W. Thompson, Coupled thermochemical, isotopic evolution and heat transfer simulations in highly irradiated UO₂ nuclear fuel, *Journal of Nuclear Materials* 441 (2013) 240–251.

- [13] S. Simunovic, S. L. Voit, T. M. Besmann, Oxygen diffusion model using the Thermochemica module in MOOSE/BISON, Tech. Rep. ORNL/TM-2014/293, Oak Ridge National Laboratory, Oak Ridge, TN (United States) (2014).
- [14] S. Simunovic, T. M. Besmann, S. L. Voit, Benchmark problem for calculating oxygen potential in high burnup LWR fuel using the Thermochemica module in MOOSE/BISON, Tech. Rep. ORNL/TM-2014/529, Oak Ridge National Laboratory, Oak Ridge, TN (United States) (2014).
- [15] S. Simunovic, T. M. Besmann, Coupling of thermochemistry solver Thermochemica with MOOSE/BISON, Tech. Rep. ORNL/TM-2015/322, Oak Ridge National Laboratory (ORNL) (2015).
- [16] S. Simunovic, T. M. Besmann, E. Moore, M. Poschmann, M. H. Piro, K. T. Clarno, J. W. McMurray, W. A. Wieselquist, Modeling and simulation of oxygen transport in high burnup LWR fuel, *Journal of Nuclear Materials* (2020) 152194.
- [17] M. Poschmann, M. H. Piro, T. M. Besmann, K. T. Clarno, S. Simunovic, Thermochemically-informed mass transport model for interdiffusion of u and zr in irradiated u-pu-zr fuel with fission products, *Journal of Nuclear Materials* (2021) 153089.
- [18] Oak Ridge National Laboratory, Oak Ridge, TN (United States), TRANSFORM, <https://github.com/ORNL-Modelica/TRANSFORM-Library> (2021).

- [19] M. Poschmann, M. Piro, S. Simunovic, Acceleration of Thermochemical calculations in BISON, Report ORNL/TM-2020/1473, Oak Ridge National Laboratory, Oak Ridge, TN (United States) (2020).
- [20] O. Hermann, R. Westfall, ORIGEN-S: SCALE system module to calculate fuel depletion, actinide transmutation, fission product buildup and decay, and associated radiation source terms, Tech. Rep. ORNL/NUREG/CSD-2/V2/R6, Oak Ridge National Laboratory (1998).
- [21] R. Serrano-López, J. Fradera, S. Cuesta-López, Molten salts database for energy applications, *Chemical Engineering and Processing: Process Intensification* 73 (2013) 87–102.
- [22] W. Grimes, D. Cuneo, F. Blankenship, G. Keilholtz, H. Poppendick, M. Robinson, Chemical aspects of molten fluoride salt reactor fuels, *Fluid-Fueled Reactors* (1958) 569.
- [23] M. S. Greenwood, B. Betzler, Modified point-kinetics model for neutron precursors and fission product behavior for fluid-fueled molten salt reactors, *Nuclear Science and Engineering* 193 (4) (2019) 417–430.
- [24] C. W. Forsberg, Molten-salt-reactor technology gaps, in: *Proc. 2006 International Congress on Advances in Nuclear Power Plants (ICAPP'06)*, Citeseer, 2006, pp. 4–8.
- [25] C. Guéneau, J.-C. Dumas, M. H. Piro, 11 - In-reactor behavior, in: M. H. Piro (Ed.), *Advances in Nuclear Fuel Chemistry*, Woodhead Publishing Series in Energy, Woodhead Publishing, 2020, pp. 419–467.

- [26] M. Kurata, M. Osaka, D. Jacquemain, M. Barrachin, T. Haste, 14
- Advances in fuel chemistry during a severe accident: Update after
Fukushima Daiichi Nuclear Power Station (FDNPS) accident, in: M. H.
Piro (Ed.), *Advances in Nuclear Fuel Chemistry*, Woodhead Publishing
Series in Energy, Woodhead Publishing, 2020, pp. 555–625.