Molten Salt Reactor PROGRAM

Update on Molten Salt Database-Thermochemical (MSD-TC)

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Molten Salt Reactor Program – Annual Review

April 21

Argonne NATIONAL LABORATORY · Idaho National Laboratory · Lawrence Livermore National Laboratory · Los Alamos NATIONAL LABORATORY · Oak Ridge National Laboratory · Pacific Northwest NATIONAL LABORATORY · Sandia National Laboratories · U.S. Department of Energy, Office of Nuclear Energy

Continual Database Expansion and Refinement Supports MSR Technology Development: *MSD-TC*

- *MSD-TC* provides a library of Gibbs energy functions and parameters for relevant solution models and their components for many salt systems of interest
  - Contains fuel/coolant compositions, fission products, additional actinides, corrosion products, and potential contaminants
  - Adopts a format that allows use with NEAMS codes including those being developed for MSR applications, allowing direct application of *MSD-TC*

- Base salt systems adopted are those detailed in the U.S. DOE MSR program roadmap of 2020*

$NaCl\text{-}ZrCl_4\text{-}UCl_3\text{-}PuCl_3$
$NaCl\text{-}KCl\text{-}AlCl_3\text{-}UCl_3\text{-}PuCl_3$
$NaCl\text{-}ThCl_4\text{-}PuCl_3\text{-}UCl_3$
$NaCl\text{-}MgCl_2\text{-}UCl_3\text{-}PuCl_3$

$FLiBe\text{-}UF_4\text{-}ZrF_4$
$LiF\text{-}NaF\text{-}ThF_4$
$NaF\text{-}BeF_2\text{-}UF_4$

***Roadmap for thermal property measurements of Molten Salt Reactor systems*, ORNL Report, March 2020, ORNL/SPR-2020/1865.**

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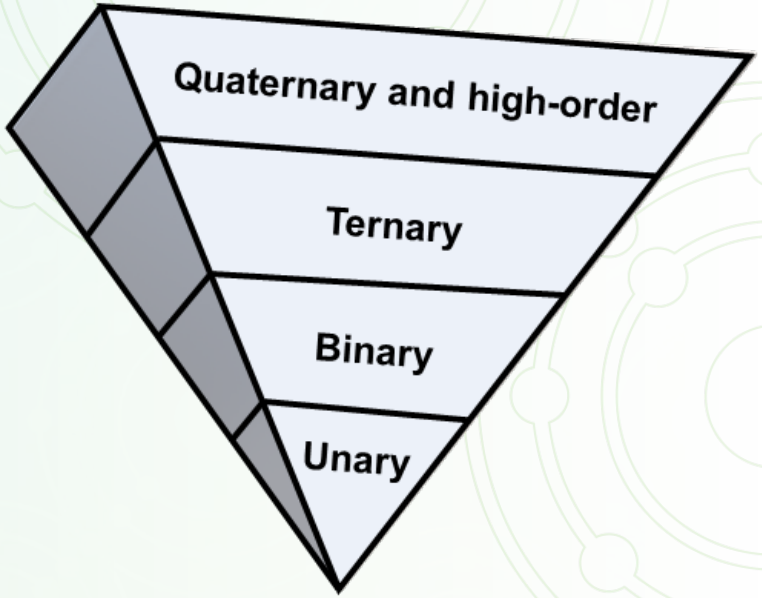
MSD-TC is a Self-consistent Molten Salt Thermochemical Database Built Up From Simple to Complex Salt Systems

- New/revised functions obtained using Computer CALculation of Phase Diagrams (CALPHAD) methodology
- Resultant Gibbs energy of each phase represented as a function of temperature, pressure, and composition
  - Modified Quasi-chemical Model in the Quadruplet Approximation (MQMQA) used for molten salts
  - Solid solution phases treated using sublattice approaches
- Equilibrium state calculated by Gibbs energy minimization codes



CALPHAD Inverted Pyramid

$$\Delta G_{solution}(\mathrm{T}) = \sum_{i=1}^{n} x_i \Delta G_i^{\circ}(\mathrm{T}) + \mathrm{RT} \sum_{i=1}^{n} x_i \ln(x_i) + \Delta G^{ex}(T)$$

Ideal Gibbs energy of mixing

Excess Gibbs energy of mixing

Gibbs energy of pure components

No interaction between solution components

Adjustable parameters model interactions by fitting to phase equilibria and other data

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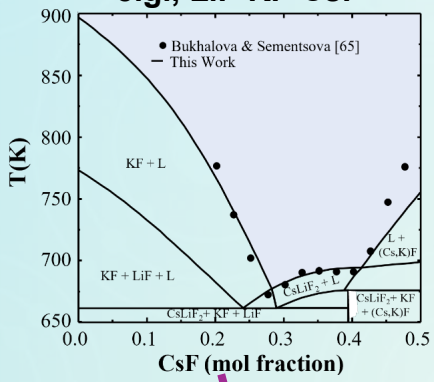
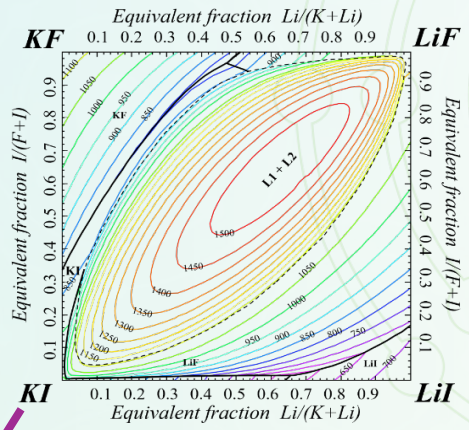
Models for Li, K, Cs | F, I Reciprocal Salt

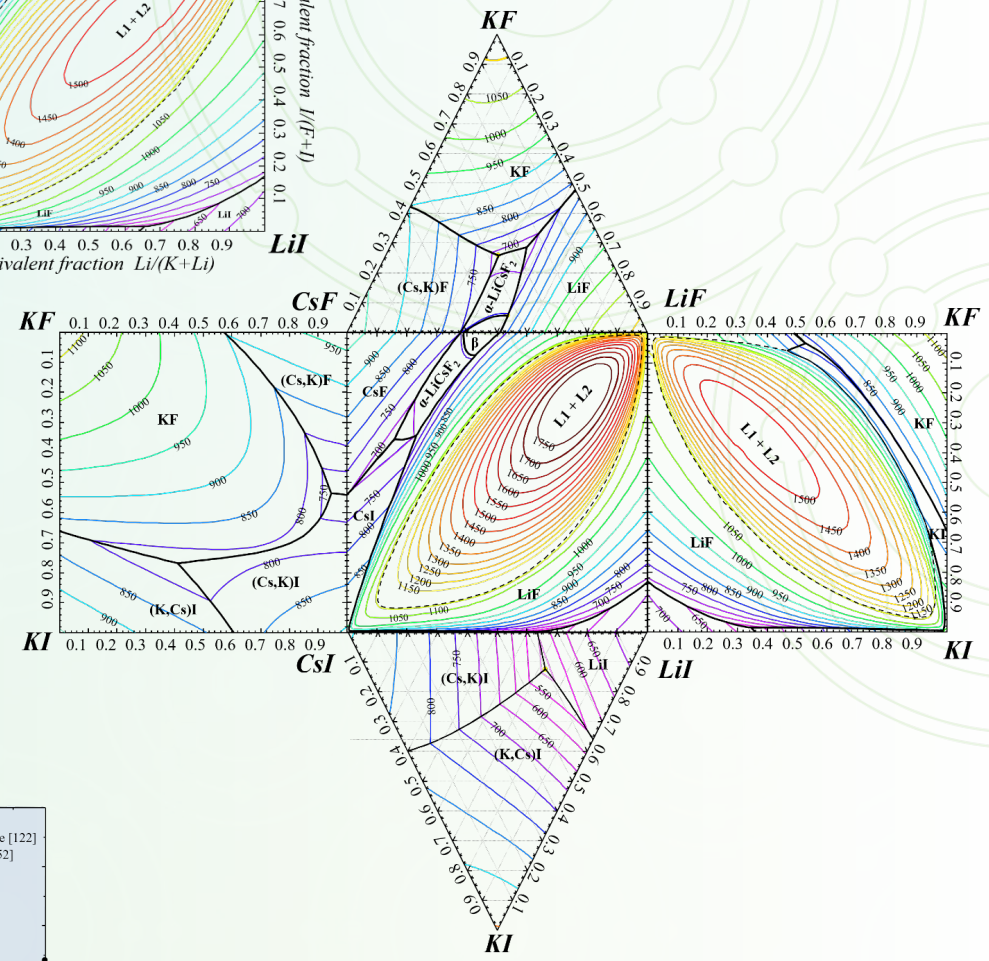
Additive Psuedo-Ternaries
e.g., LiF-KF-CsF



Reciprocal Ternaries
e.g., Li, K | F, I

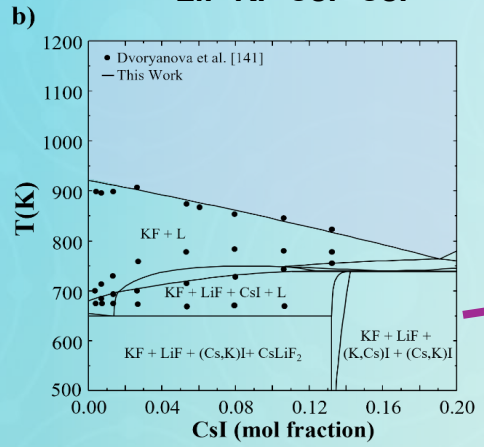


Unfolding the prism reveals the modeled relationship among salt components



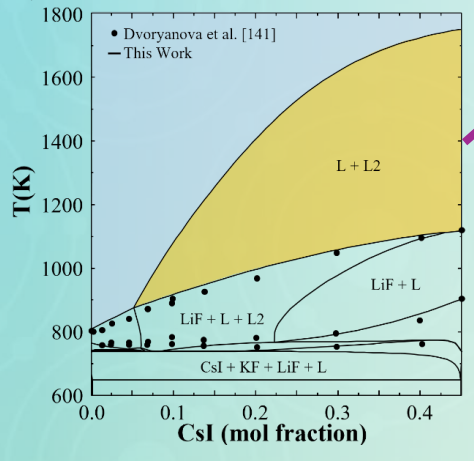
Reciprocal Quaternary Internal Sections
LiF-KF-CsF-CsI

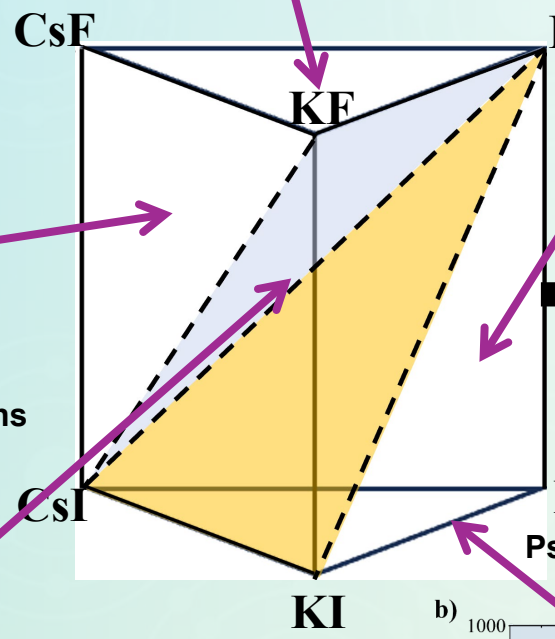
b)



Reciprocal Quaternary Internal Sections
LiF-KF-CsI

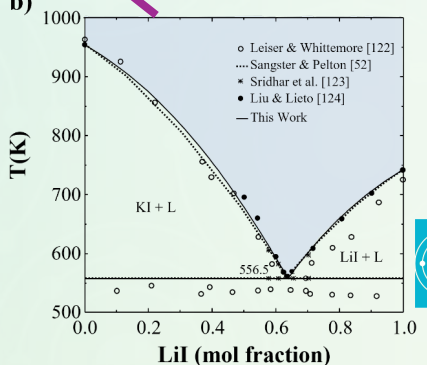
a)





Psuedo-Binaries
e.g., LiI-KI

b)



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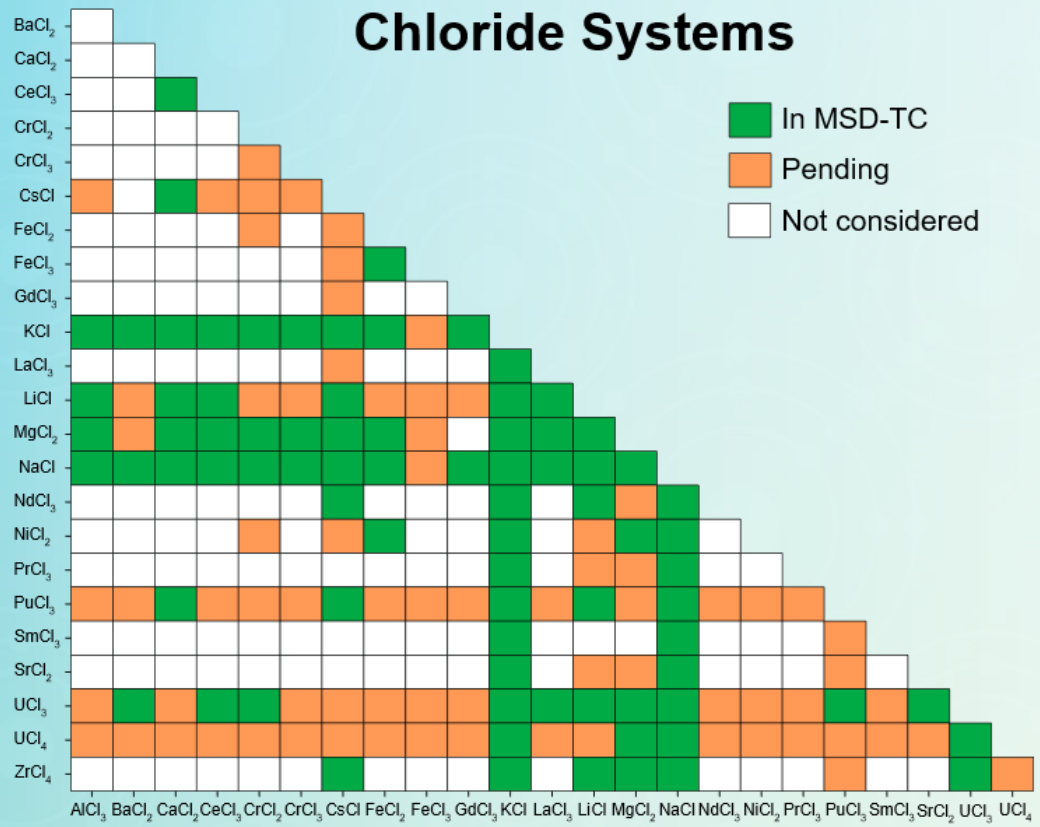
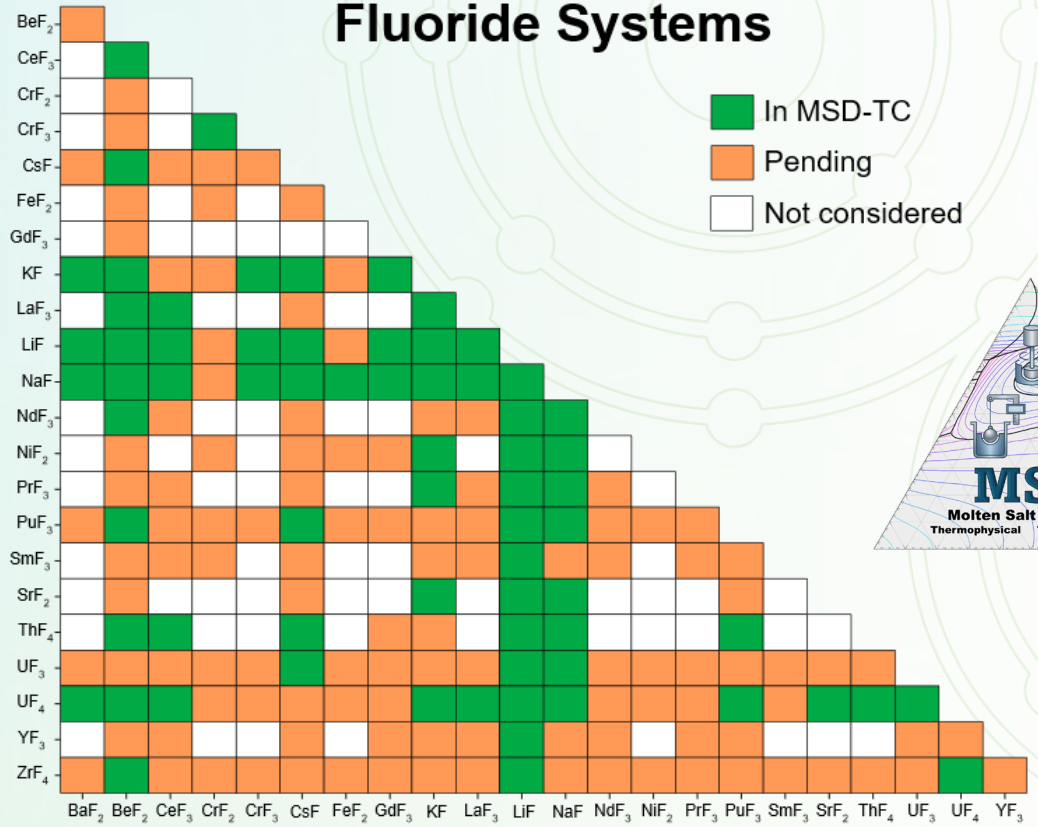
Content of Current *MSD-TC* Ver. 4.1

Pseudo-binary System Content Matrices

Chloride Systems



Fluoride Systems



29 salt cations

170 pseudo-binary systems

54 pseudo-ternary systems

28 reciprocal salts with iodine

Fe-Cr-Ni-Mo alloy phase systems

Ru-Rh-Pd-Mo-Tc noble metal phase systems

Kr, Xe, Ne, Ar, He inert gases

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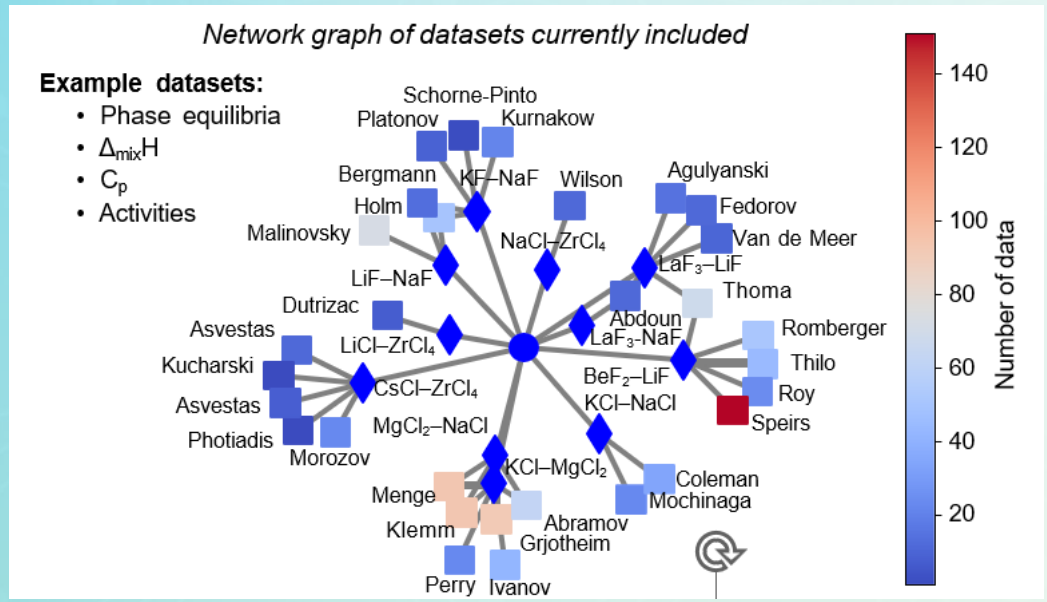
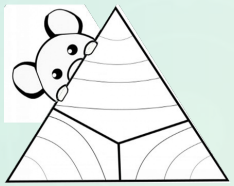
Data Management and Finding and Propagating Uncertainty

Data Systematically Digitized and Centrally Stored

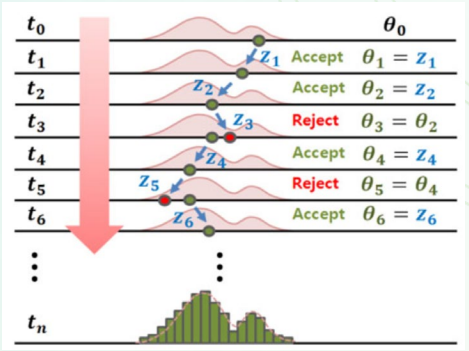


Molten-salt
Open
Unified
Set of
Experiments

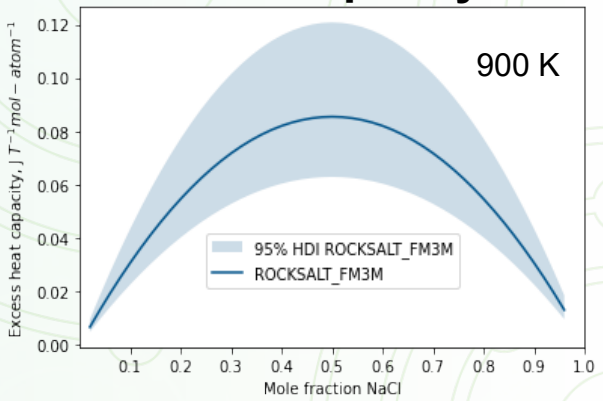


Digitized datasets are stored as versatile JSON files:
- Include metadata and DOI links (where available)
- Standardized and machine-readable for easy integration

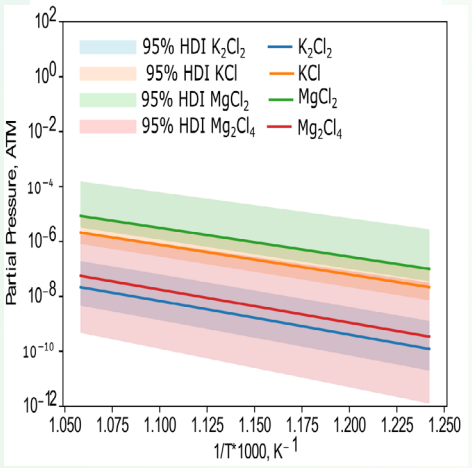
Bayes' Theorem



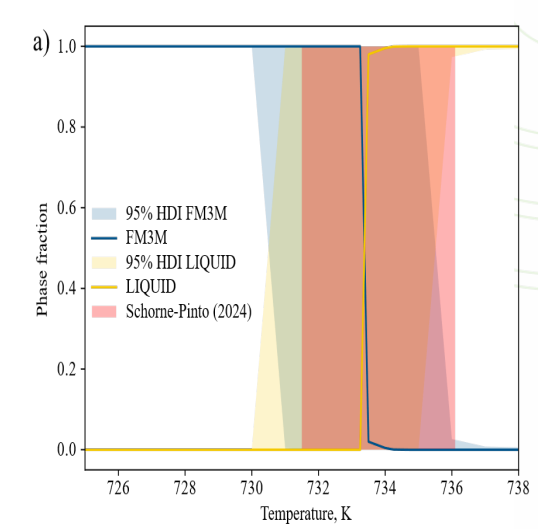
Heat Capacity



Partial Pressures



Phase Equilibria



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What's New in MSD-TC Ver. 4.1, and What's Removed

- New
  - Revised CsCl–$MgCl_2$–NaCl model to include new, original thermochemical and phase equilibria measurements
  - New assessments of $SmCl_3$, $GdCl_3$, $PrCl_3$–(NaCl, KCl)
  - New assessments of SmF_3, GdF_3, PrF_3–(KF ,LiF, NaF)
  - More recent and accurate thermodynamic models and values for the noble metal systems replace previous entries
  - Alloy and intermetallic systems containing Cr-Ni-Fe-Mo added to allow direct computing of potential corrosion behavior
  - Gibbs energy functions of the noble gases have been included
- Removed
  - Review of information for systems with RbF and RbCl was felt to be insufficiently supported

FeF_2-KF	NaF-RbF	LiCl-RbCl
KF-RbF	LiF-NaF-RbF	$MgCl_2$-RbCl
LaF_3-RbF	LiF-KF-RbF	NaCl-RbCl
PuF_3-RbF	CsCl-RbCl	$PuCl_3$-RbCl
LiF-RbF	KCl-RbCl	

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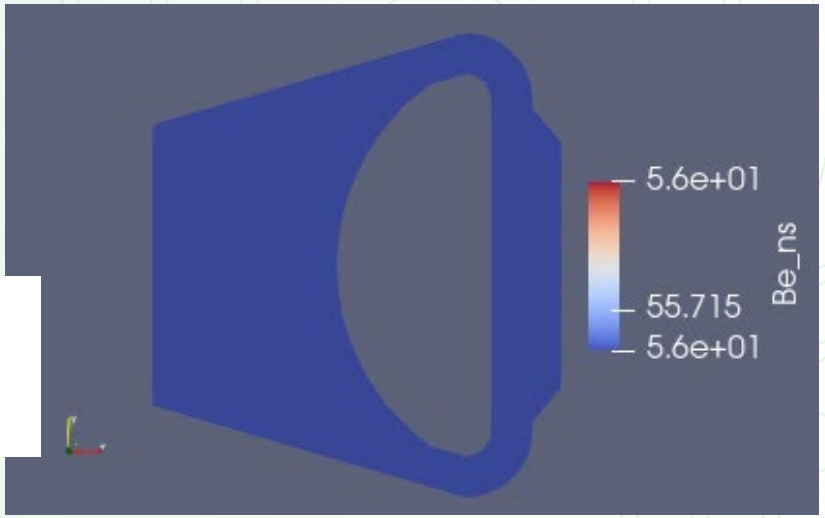
FY26 Milestone Activity

Developing thermochemical models via reported properties and original synthesis and measurement

- Rb with MSR solvent salts and iodine
  - Experimental measurements required for endmembers
- Cr^{+2} with LiF modeled using extant data
- $Cr^{+2\ or\ +3}$ with UF_4
  - Successfully synthesized CrF_2 with DSC measurements underway
  - Experimental phase equilibria and thermal properties of UF_4-CrF_3 and UF_4-CrF_2 will follow
- $Cr^{+2\ or\ +3}$ with UCl_3
  - Efforts problematic as UCl_3 dissociates to U + UCl_4 during synthesis of phase mixtures
  - Synthesis route reacting UCl_4 with Si found to be successful
- $NiCl_2$ with UCl_3 work completed
- NiF_2 with BeF_2 and UF_4
  - Currently synthesizing NiF_2 with planned thermal property measurements for NiF_2 + UF_4
  - Utilizing computational and reported experimental values to determine thermal properties of for NiF_2 + BeF_2

Application Example: MSD-TC with Thermochimica Coupled to Navier-Stokes Module in the MOOSE Framework

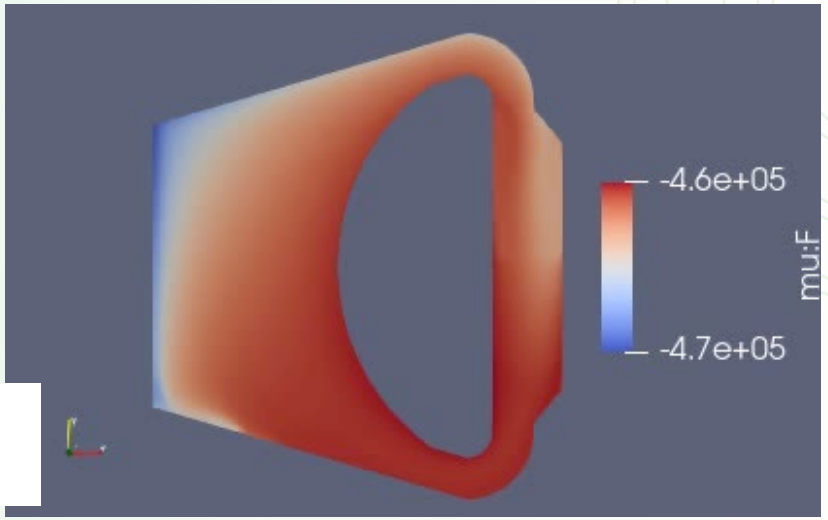
Redox control via reducing metal (beryllium) addition to MSRE



Mixing of beryllium added to lower plenum (Be distribution in mols)

Code applications for MSD-TC via Thermochimica

- Mole: Multi-species/phase reactive mass transport
- Pronghorn: Multi-dimensional thermal-hydraulics for intermediate-fidelity CFD
- SAM: Transient analysis using 1D flow networks to represent fluid systems with general species transport capability



Resultant reduction in fluorine potential (J/mol)

Walker et. al (2023) INL/RPT-23-74376

Courtesy of M. Tano, S. Walker, P. Bajpai, D. Schwen, Idaho National Laboratory

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FY 25-26 Publications on Thermophysical and Thermochemical Efforts

- *Thermodynamic Assessment of the Na, K, Cs, Mg | Cl, I Reciprocal System, C.* M. Dixon, et al., J. Nucl. Sci. Eng., 2026, in press.
- *Understanding the structure and thermal stability of Cs3UCl6 phase in the CsCl-UCl3 system,* A. Padinhare Manissery, et al., Inorganic Chemistry, in press.
- *Thermodynamic assessment of SmF_3 with LiF, NaF, and KF (FLiNaK) for Molten Salt Reactors,* J. A. Wilson, et al., ACS Omega, in press.
- *MOLTSA: An R Shiny platform for molten-salt thermochemical data management, analysis, and CALPHAD-ready workflows,* J. A. Wilson, et al., Journal of Open Research Software, in press
- *Thermodynamic assessment of the Li, Na, K, Cs | F, I reciprocal salt for MSR applications,* C. M. Dixon, et al., J. Chem. Thermo., 211 (2025) 107548.
- *Round Robin Measurements of Molten Salt Properties for LiF-NaF-KF (FLiNaK) and NaCl-KCl Mixtures*, Troy Munro,et al., J. Chem. Eng. Data, 71, (4) (2025) 1541.
- *Thermodynamic Properties of $ZrCl_4$ with LiCl, NaCl, KCl, CsCl, $MgCl_2$, and UCl_3 for Molten Salt Reactor Applications,* Jack A. Wilson, et al., Journal of Molecular Liquids, 437 (2025) 128578.

FY 25-26 Publications on Thermophysical and Thermochemical Efforts

- *Structural coherence model for predicting molten salt thermal conductivity informed by the pair distribution function*. J. Numbers, et al. *Journal of Molecular Liquids*, (2026) 129502.
- *Toward a Generalizable Prediction Model of Molten Salt Mixture Density with Chemistry-Informed Transfer* Learning, J. Barra, J., et al., Chem. Phys. Chem, 26, (23) (2025) e202500273.
- *Reference Correlations for the Density and Viscosity of Molten Alkali and Alkaline Earth Fluoride* Salts. A. Birri, et al., Journal of Physical and Chemical Reference Data, 54, (2) (2025)
- *Molten Halide Salt Surface Tension: Methods and Correlations*, R. Chesser, Int. J. Thermophys., 47 (2026) 80.
- *An Overview of the Molten Salt Thermal Properties Database–Thermophysical, Version 4.0 (MSTDB-TP V.4.0)*. R. Chesser, et al., ORNL/TM-2025/4159(2025).

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Questions?

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