Molten Salt Reactor
PROGRAM

Update on Molten Salt Database—Thermophysical (MSD-TP)

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Molten Salt Reactor Program – Annual Review

April 21

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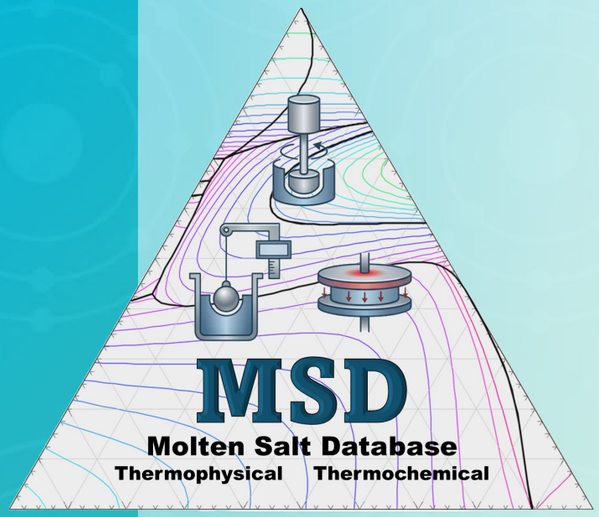
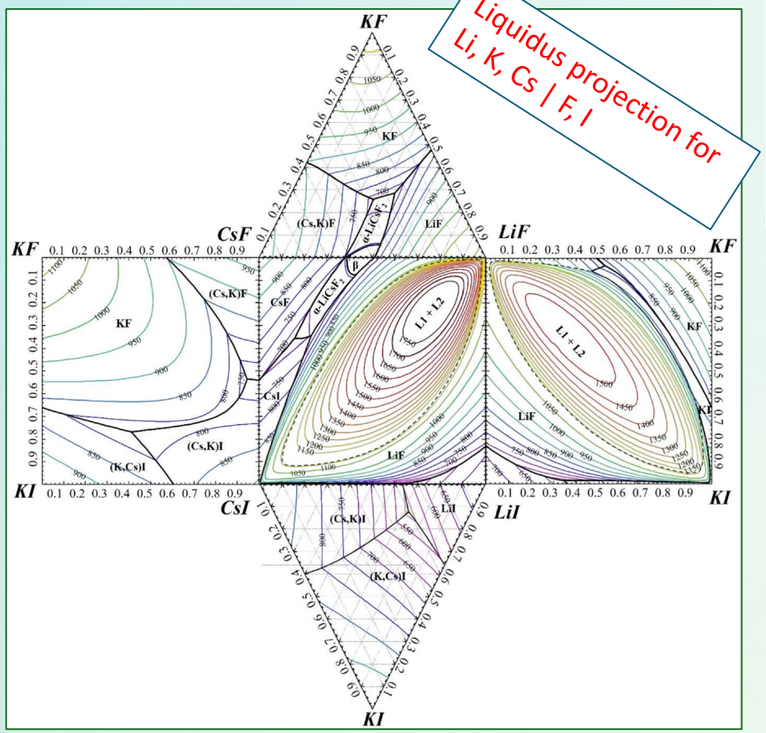
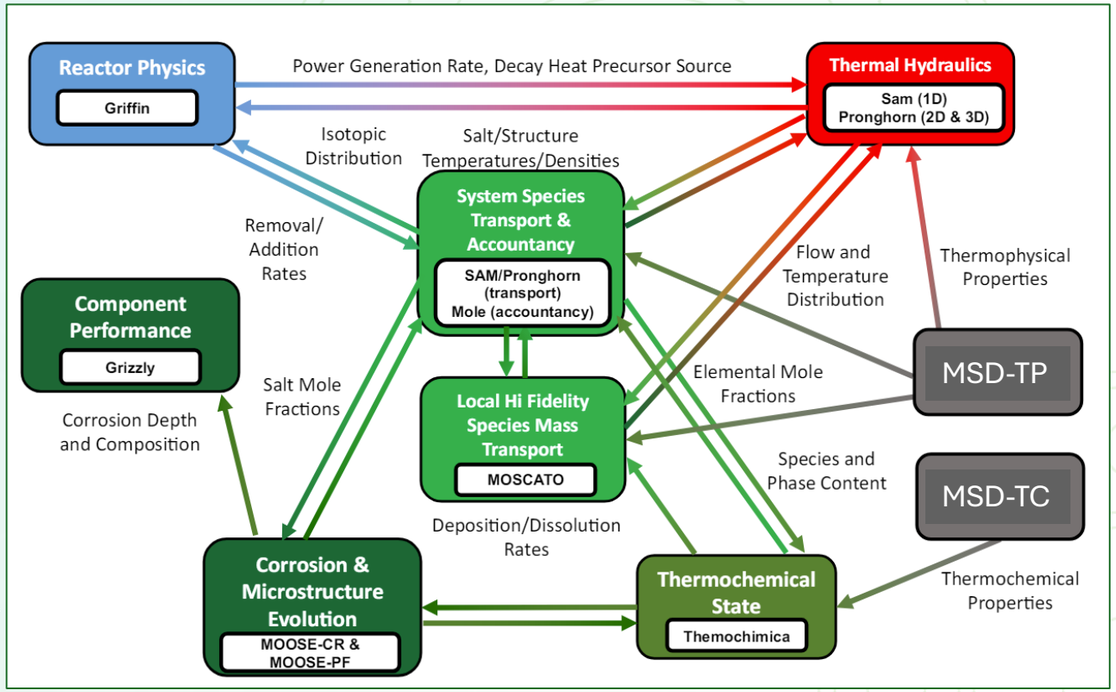
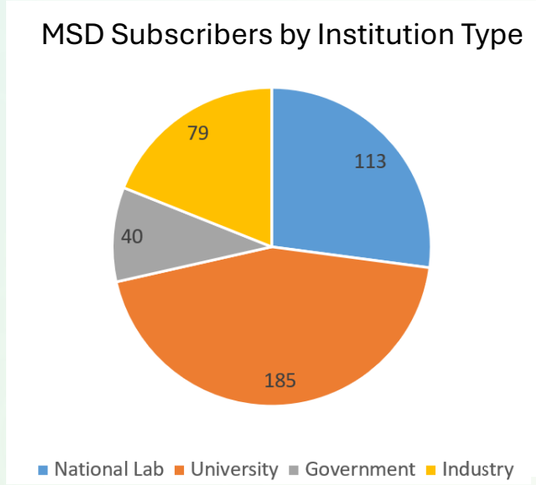
Overview of MSD

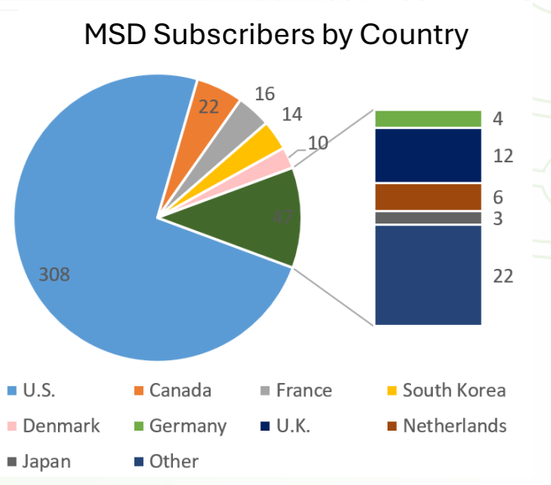
- The Molten Salt Database–Thermochemical (MSD-TC) and Molten Salt Database–Thermophysical (MSD-TP) are available via the ORNL/ITSD Gitlab Server.











[1] INL/RPT-22-70694
[2] ORNL/TM-2025/4159
[3] Dixon, Clara M., et al. The Journal of Chemical Thermodynamics (2025): 107548.

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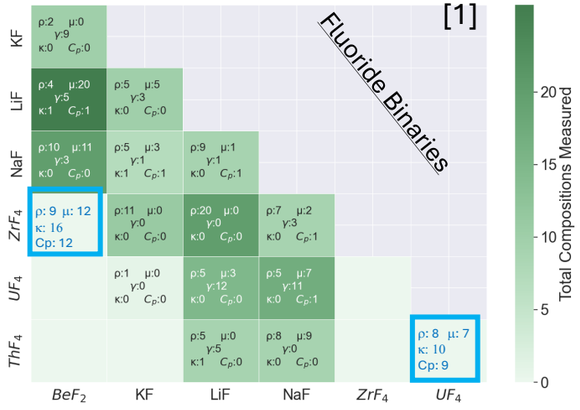
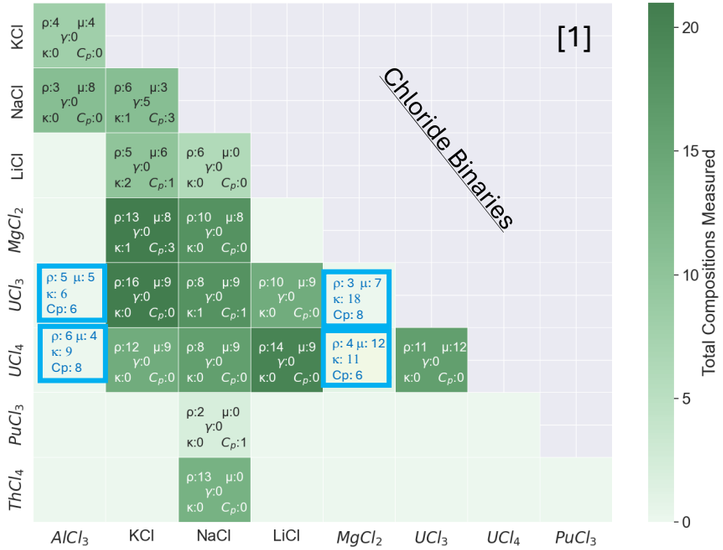
MSD-TP 4.0 Overview

- As per the current version release (**4.0**) There are **976 entries**
  - Newest version contains surface tension data
  - **MSD-TP is driven by a roadmap laid out in 2020: ORNL/SPR-2020/1865**
  - **In blue: literature entries using LLM's (Zhang, Glezakou)**





Version:	1.0	2.0	2.1	3.0	3.1	4.0
Release Date:	Feb-21	Mar-22	Dec-22	Mar-24	Dec-24	Oct-25
Number of Entries:	62	273	448	799	820	976
RK Binary System Characterizations:	0	0	21	29	47	47
Saline Integration of RK Density:	No	No	Yes	Yes	Yes	Yes
Saline Integration of RK Viscosity:	No	No	No	No	Yes	Yes
Number of Properties Considered:	4	4	4	4	4	5

Pure Compounds

Salt	ρ	μ	κ	c_p	γ
AlCl3	1	1	0	1	0
BeCl2	1	0	0	0	0
BeF2	1	1	1	1	0
CaCl2	1	1	1	1	1
CaF2	1	1	1	1	1
GdCl3	1	1	0	0	1
GdF3	0	0	0	0	0
KCl	1	1	1	1	1
KF	1	1	1	1	1
LaCl3	1	1	0	0	1
LaF3	1	0	0	1	0
LiCl	1	1	1	1	1
LiF	1	1	1	1	1
MgCl2	1	1	1	1	1
MgF2	1	1	1	0	1
NaCl	1	1	1	1	1
NaF	1	1	1	1	1
NdCl3	1	1	0	0	1
NdF3	0	0	0	1	0
NpCl3	0	0	0	0	0
NpF3	0	0	0	0	0
PuCl3	0	0	0	1	0
PuF3	0	0	0	1	0
SrCl2	1	1	1	0	1
SrF2	1	1	1	0	1
ThCl4	1	0	0	0	0
ThF4	1	0	0	0	1
UCl3	1	1	0	1	1
UCl4	1	1	0	0	1
UF3	0	0	0	1	0
UF4	1	1	0	1	1
ZrCl4	1	1	0	0	0
ZrF4	1	0	0	0	1
RbCl	0	0	0	0	1
CsCl	0	0	0	0	1
BaCl2	0	0	0	0	1
PrCl3	0	0	0	0	1
RbF	0	0	0	0	1
CsF	0	0	0	0	1
BaF2	0	0	0	0	1
UF6	0	0	0	0	1

Ternaries

Salt	ρ	μ	κ	c_p	γ
AlCl3-LiCl-NaCl	10	10	0	0	0
BeF2-KF-NaF	1	1	0	1	0
BeF2-LiF-NaF	5	4	0	5	0
BeF2-LiF-ThF4	3	2	0	0	44
BeF2-LiF-UF4	36	38	2	0	1
BeF2-LiF-ZrF4	1	0	0	0	0
BeF2-NaF-UF4	78	70	0	0	1
KCl-LiCl-NaCl	4	0	0	0	0
KCl-LiCl-UCl3	18	0	0	0	0
KCl-LiCl-UCl4	18	0	0	0	0
KCl-MgCl2-NaCl	1	1	1	1	0
KCl-NaCl-UCl3	18	20	0	1	0
KCl-UCl3-UCl4	32	0	0	0	0
KF-LiF-NaF	1	1	1	1	1
KF-MgF2-NaF	1	0	1	1	0
KF-NaF-UF4	4	2	3	3	0
KF-NaF-ZrF4	1	1	0	1	0
NaCl-PuCl3-UCl3	3	0	0	0	0
MgCl2-NaCl-PuCl3	2	0	0	0	0
LiCl-NaCl-UCl3	18	0	0	0	0
LiCl-NaCl-UCl4	18	0	0	0	0
LiCl-UCl3-UCl4	21	0	0	0	0
LiF-NaF-ZrF4	10	1	1	2	11
LiF-ThF4-UF4	1	0	0	0	0
NaCl-UCl3-UCl4	21	40	0	0	0
NaF-UF4-ZrF4	5	4	0	6	0
RbF-UF4-ZrF4	2	2	0	2	0
CaCl2-LaCl3-NaCl	0	0	0	0	1
CaF2-LiF-NaF	0	0	0	0	1
KF-LiF-ZrF4	0	0	0	0	1

Quaternaries

Salt	ρ	μ	κ	c_p	γ
BeF2-LiF-NaF-UF4	1	1	0	1	0
BeF2-LiF-ThF4-UF4	1	1	1	1	32
BeF2-LiF-UF4-ZrF4	1	0	1	0	0
BeF2-NaF-UF4-ZrF4	1	0	0	0	0
KF-LiF-NaF-UF4	2	2	0	2	0
KF-NaF-UF4-ZrF4	0	0	0	2	0
LiF-NaF-UF4-ZrF4	1	1	0	2	0
BeF2-NaF-ThF4-UF4	0	0	0	0	1

[1] ORNL/TM-2025/4159

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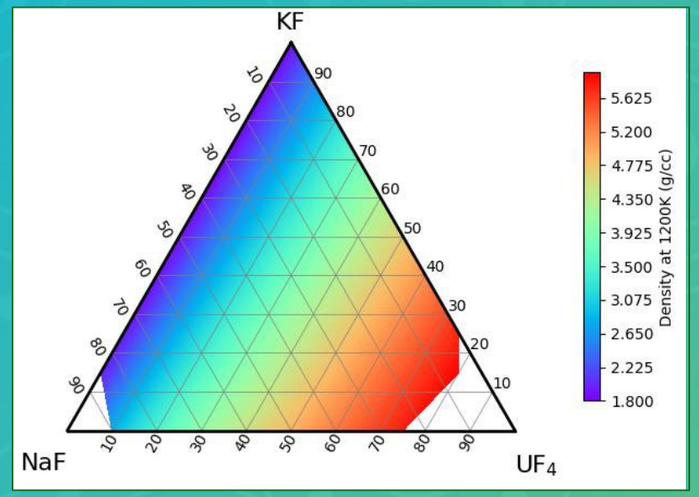
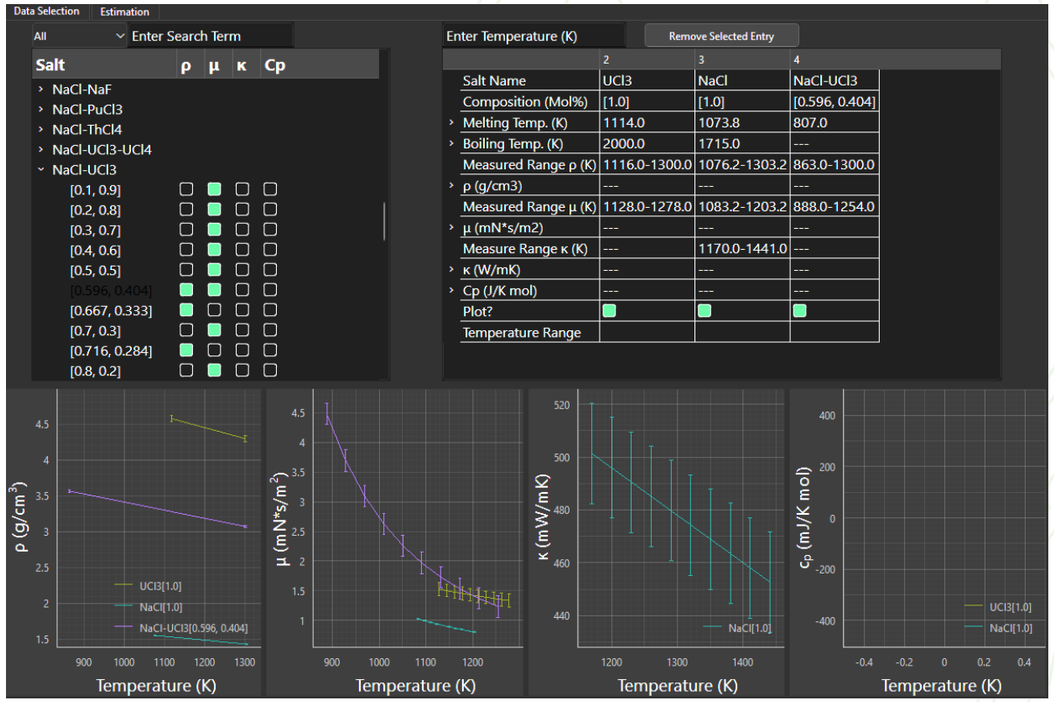
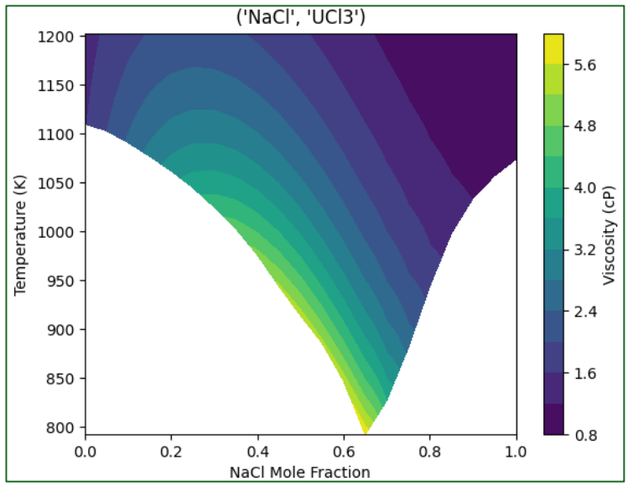
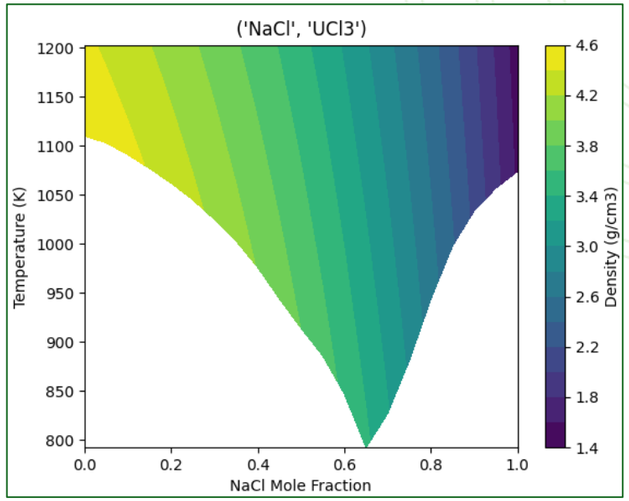
Interfaces: Saline, GUI

- Saline is a stable c++ API with a python wrapper available. Implemented in MOOSE as an object.
  - Ideal for code integration, accessing data rapidly
- GUI can be downloaded as a .exe file
  - Predictive models are outputted over ranges deemed valid via thermochimica-generated look-up table









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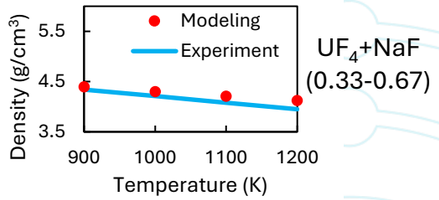
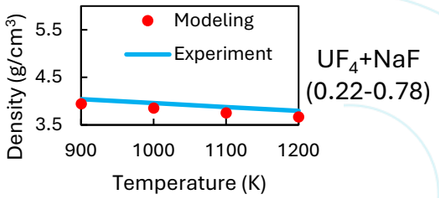
Bridging the gaps; a multifaceted solution

- Several gaps to fill in the database; how do we address this?
- Multifaceted approach to solving this going forward:
  - **Traditional solution models (such as RK) to interpolate and extrapolate [1]**
  - **Transfer Learning with ML [2]**
  - **Direct calculation with MD [3,4]**
  - **Experimental and theoretical collaboration through the MSR program [5]**
  - **Other theoretical approaches (such as kinetic theory)**

UF_4+NaF [4]

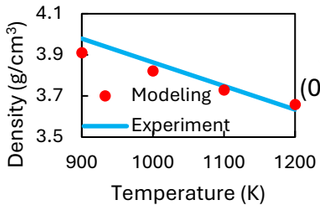


UF_4+NaF (0.33-0.67)

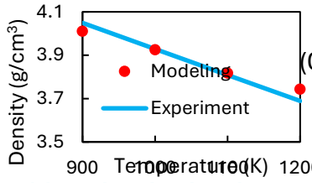


UF_4+NaF (0.22-0.78)

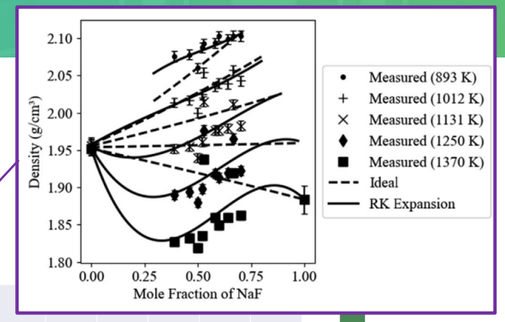
UF_4+NaF+KF [4]

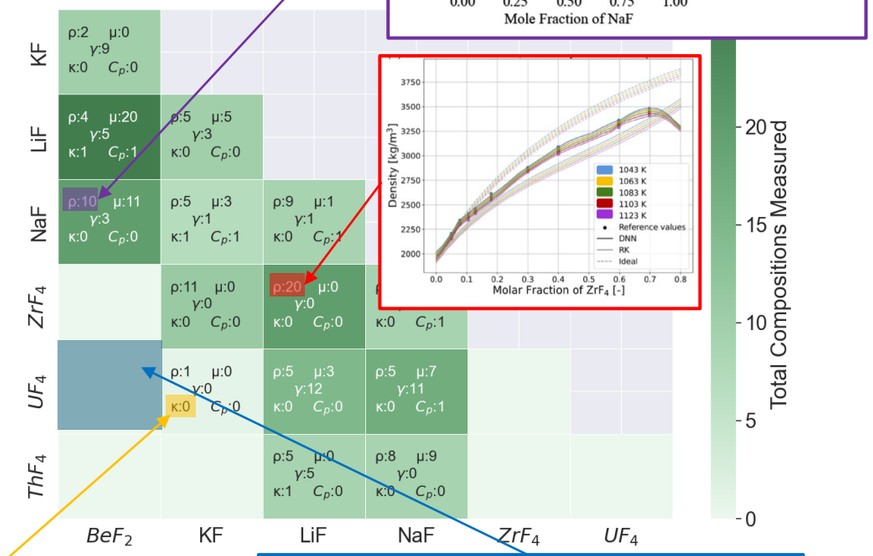


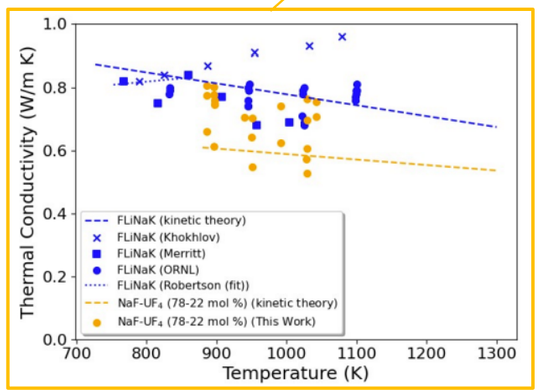
UF_4+NaF+KF (0.27-0.47-0.26)

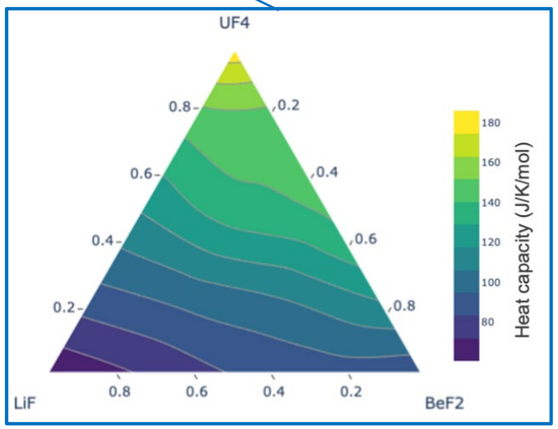


UF_4+NaF+KF (0.27-0.57-0.16)



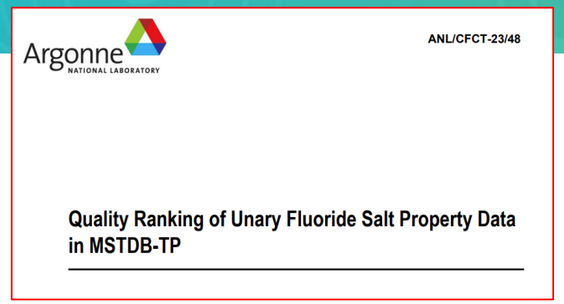




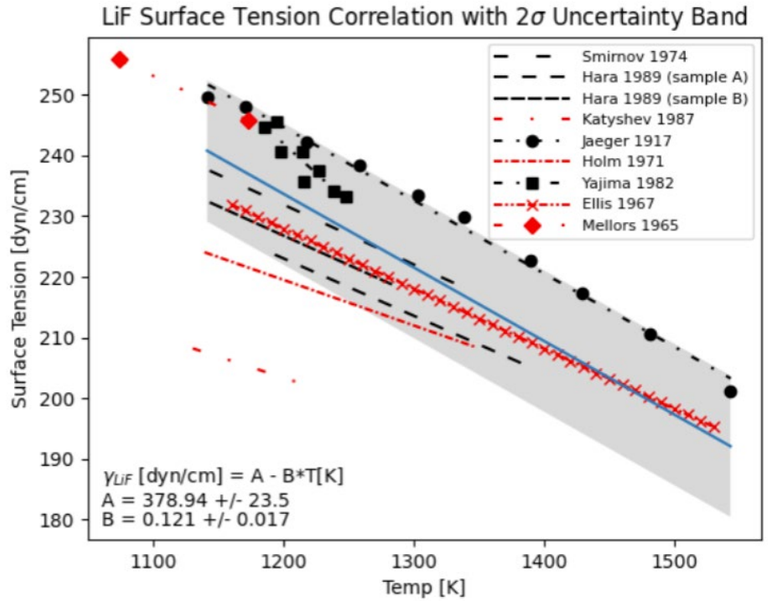


[1] Birri, Anthony, et al. Chemical Engineering Science 260 (2022): 117954.
[2] Barra, Julian, et al. ChemPhysChem 26.23 (2025): e202500273.
[3] Wang et al. "Ab-initio molecular dynamics simulations of LiF-BeF2-UF4 molten salts". LANL.
[4] Zhang, Glezakou MD properties and transport in NaF-UF4, NaF-KF-UF4, in preparation
[5] ORNL/TM-2025/4057

A note on uncertainty

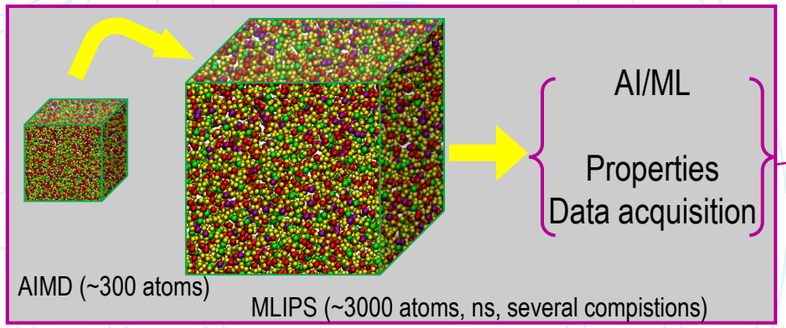


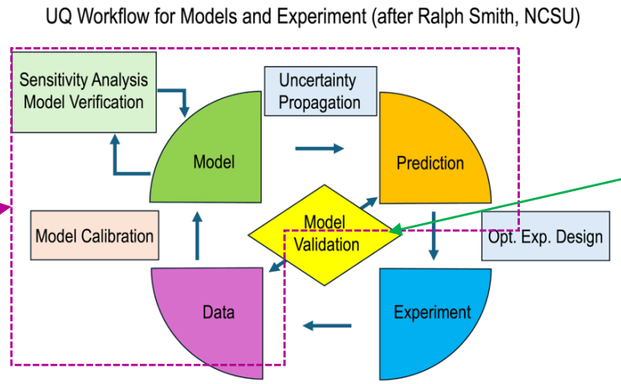
- MSD-TP currently contains experimental data, with the plan to integrate MD-generated data in the next iteration
- For experimental uncertainties, sometimes the uncertainties are well characterized
- However, sometimes data is provided without error bars; then we rely on conservative assumptions
- As we integrate MD data, we are working with experts in NEAMS to establish a strategy
  - Data quality assessments will help in this effort
- General observation: Uncertainty quantification relies on statistical methods, hence large, well-curated datasets are required [2]
  - Computed data with well-validated models can fill these gaps

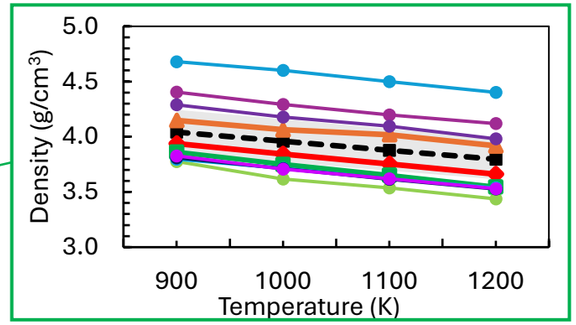


[1] Chesser et al. "Molten Salt Surface Tension - Methods and Correlations". Under review

[2] Zhang, Rousseau, Glezakou ACS Catal., 14(10), pp.8073-8086







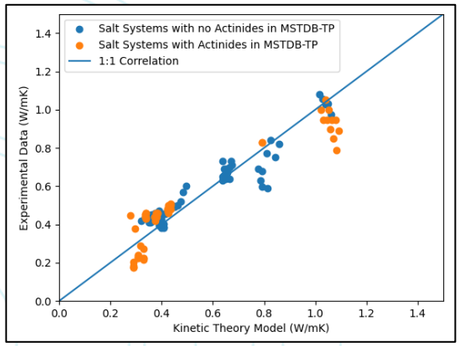
Thermal Conductivity Modeling

- The lack of experimental thermal conductivity data necessitates a more theoretical model
- We have shown that a kinetic theory provide accurate data for actinides
  - Existing frameworks underpredict thermal conductivity
- This modeling approach relies on characterizing phonon transport
  - In some cases, where MD data is sufficient, phonon transport can be characterized by PDFs

Kinetic Theory Model (purely theoretical)

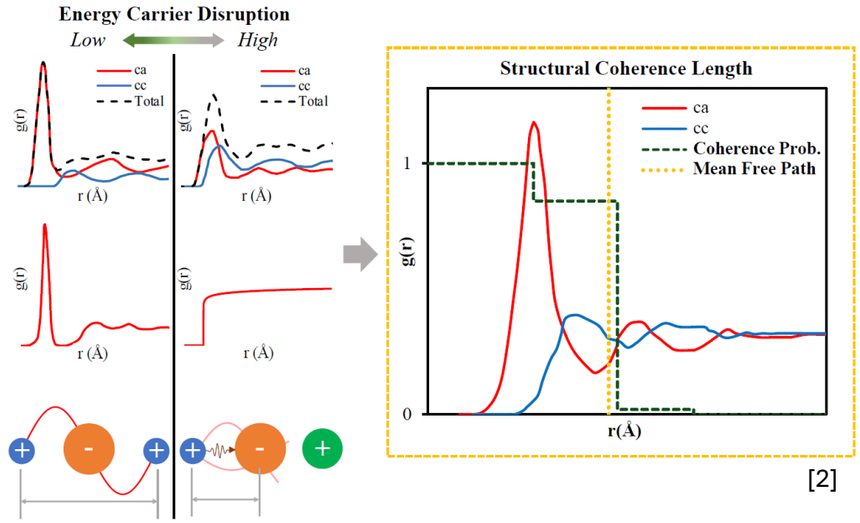
$$\kappa = K(1-\delta)k_B\left(\frac{N_A n}{V(T_m)}\right)C_0(T_m)\left(1-\alpha(T_m)\left(\gamma(T_m)+\frac{1}{3}\right)(T-T_m)\right)$$

- Scaling factor for complexation and ionic mass differences
- Boltzmann constant
- Phonon mean free path
- Group velocity
- Temperature dependence (relies on heat capacity)



[1]

Structural Coherence Model (tied to PDFs)



[2]

[1] ORNL/TM-2025/4159
[2] Numbers et al. "Structural Coherence Model for Predicting Molten Salt Thermal Conductivity Informed by the Pair Distribution Function." Under Review.

Acknowledgements

- Ted Besmann, Juliano Shorne-Pinto, and Jorge Paz Soldan Palma from USC for fruitful collaborations on MSD
- Troy Munro and Jacob Numbers at BYU for thermal conductivity modeling collaborations
- Chao Jiang and Gaoxue Wang at INL and LANL for insightful discussions regarding MD integration

This work is directly funded by the Molten Salt Reactor Program and Nuclear Advanced Modeling and Simulation Program under the Department of Energy, Office of Nuclear Energy.

Questions?

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