U.S. DEPARTMENT OF ENERGY | Office of NUCLEAR ENERGY

Molten Salt Reactor PROGRAM

Overview of MSTDB-TP

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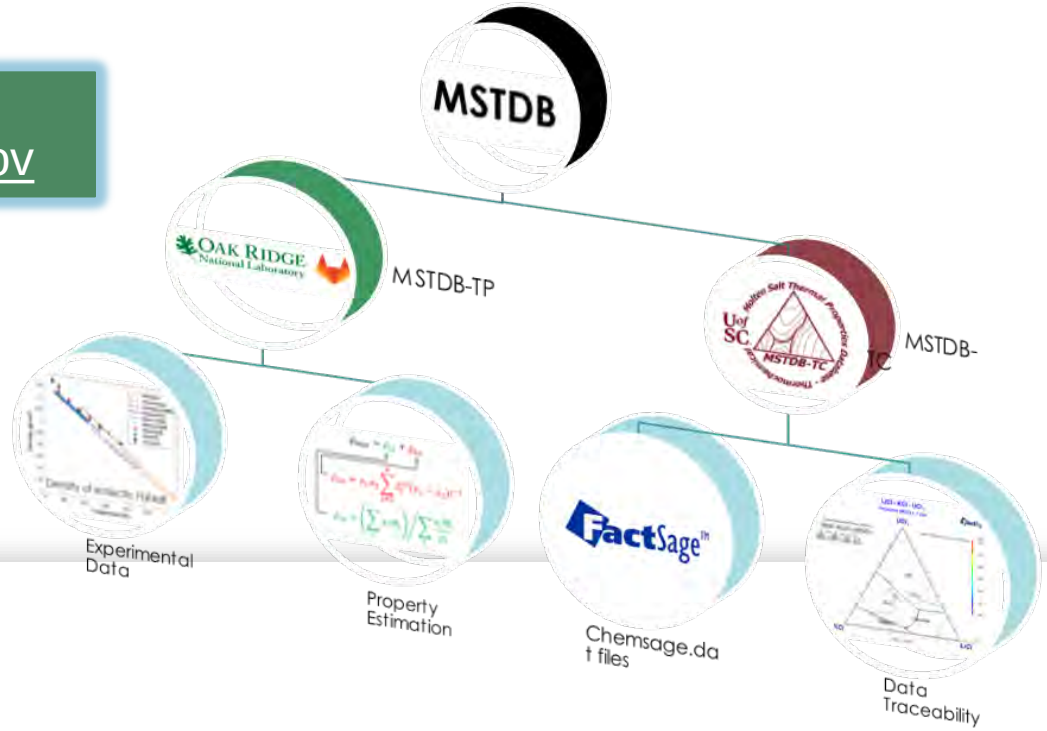
How to get Access

- **The databases and associated documents are hosted on a publicly accessible, permission-protected server at Oak Ridge National Laboratory (ORNL):**
- **https://code.ornl.gov/neams/mstdb/**
- **Access requires an ORNL XCAMS account and an MSTDB membership, which once granted will allow downloading of all files.**

Contact:
mstdb@ornl.gov



Molten Salt Thermal Properties Databases

The Molten Salt Thermal Properties Database–Thermochemical (*MSTDB-TC*) and Molten Salt Thermal Properties Database–Thermophysical (*MSTDB-TP*) databases are now available for public use. *MSTDB-TC* contains Gibbs energy models and values for molten salt components and related systems of interest with respect to molten salt reactor technology. *MSTDB-TP* consists of tabulated thermophysical properties and relations for computing properties as a function of temperature or composition.

MSTDB-TC thermodynamic information resides in files in the "Chemsage" .dat (ASC II) format for use with the FactSage® commercial package of thermodynamic codes and compatible with the open-source equilibrium code Thermochimica.

- Separate files are provided for chloride- and for fluoride-based systems.
- Changes by FactSage® developers have resulted in the need to provide files readable by FactSage® Ver. 8.0 or lower and FactSage® Ver. 8.1 or higher, as noted in the documentation that will accompany the database download.
- Additional files include those for tracing all data sources and a library of published phase diagrams together with companion *MSTDB-TC*-computed phase diagrams to allow the user to compare model results with those previously reported.

MSTDB-TP contains sets of referenced values and relations for thermophysical properties including density, thermal conductivity, viscosity, heat capacity, and related optical properties. The database is maintained as a csv file of the salt systems thermophysical property data, uncertainty (when available), and literature references.

Accessing MSTDB: The databases and associated documents are hosted on a publicly accessible, permission-protected server at Oak Ridge National Laboratory (ORNL): https://code.ornl.gov/neams/mstdb/. Access requires an ORNL XCAMS account and an MSTDB membership, which once granted will allow downloading of all files.

- XCAMS account creation
  - Go to https://xcams.ornl.gov
  - Select "I need an account."
  - Read and acknowledge the User Agreement
  - Enter your email address and username following the guidelines on the page.
  - Enter "Personal Information" and "Contact Information" per the guidelines
  - Create an XCAMS password according to the guidelines provided on the page.
  - On the final step, note the activation sequence box at mid-page. Wait until each action item turns green and the box heading reads "Transactions Complete"
  - Log into https://code.ornl.gov using your new XCAMS username and password
- Request MSTDB membership
  - Send an email to mstdb@ornl.gov with "MSTDB Access Request" as subject
  - Include your XCAMS ID and brief summary of the purpose for your request

MSTDB-TC is a copyrighted database available license-free, and cannot be sold all or in part. Development is supported by the U.S. Department of Energy, Office of Nuclear Energy Molten Salt Reactor Campaign, Nuclear Energy Advanced Modeling and Simulation Program, and Nuclear Energy University Programs. *MSTDB-TP* is a product of Department of Energy MSR-related research programs.

Contacts: *MSTDB-TC* Ted Besmann (besmann@sc.edu)
MSTDB-TP Dianne Ezell (bullnd@ornl.gov)

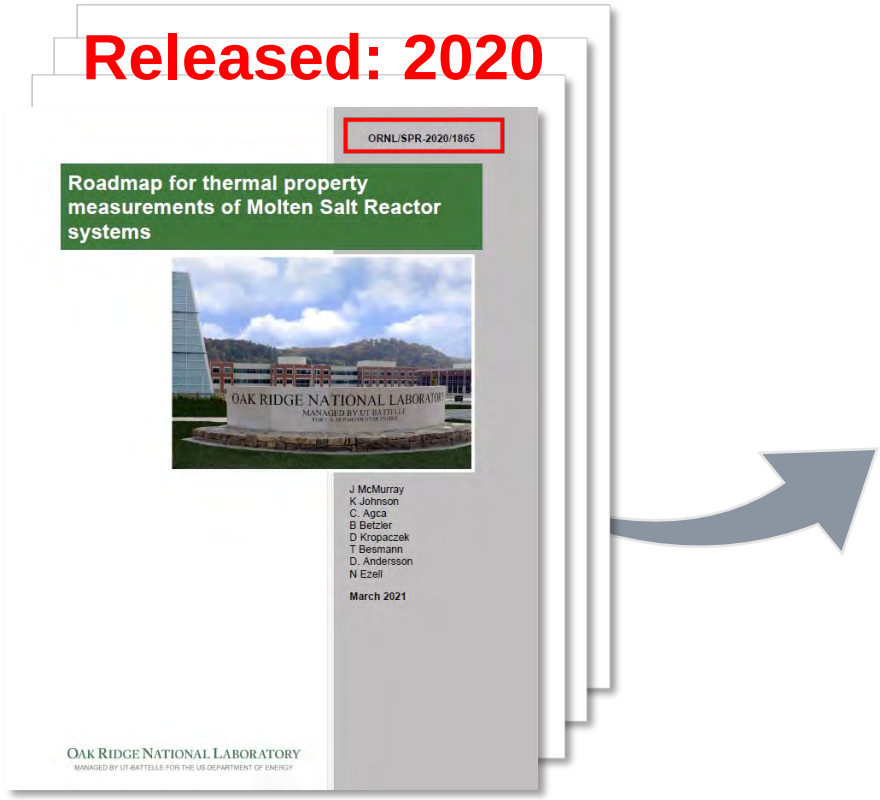
MSTDB-TP Overview

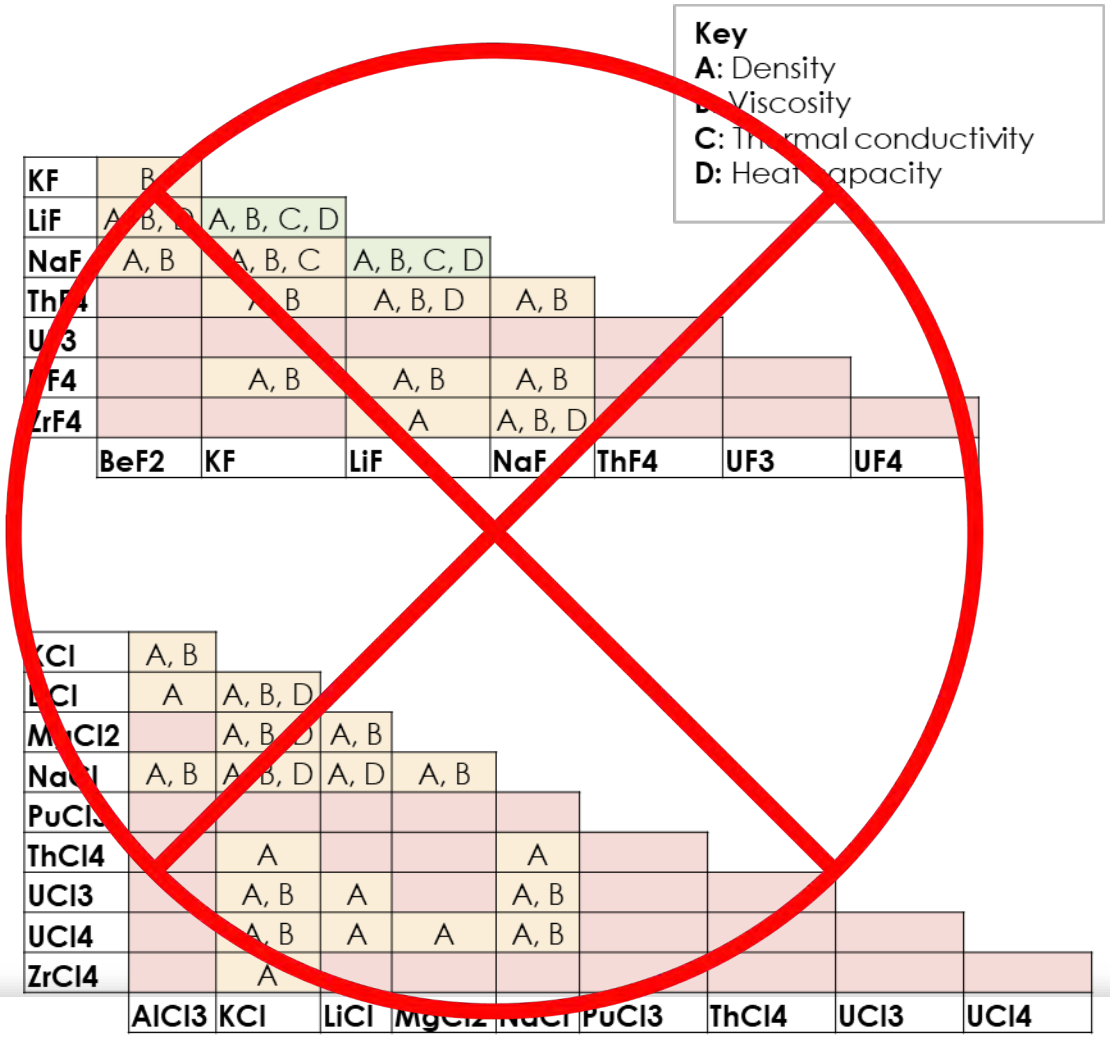
Please submit your publications with measurement data (including uncertainty)

- **The Molten Salt Thermal Property Database– Thermophysical (MSTDB-TP) contains empirical relations for the following properties:**
  - Melting and boiling points
  - Density
  - Viscosity
  - Heat Capacity
  - Thermal Conductivity
- **As per the current version release (v2.1) There are 448 entries, including:**
  - 33 pure compounds
  - 243 pseudo-binaries
  - 166 pseudo-ternaries
  - 6 pseudo-quaternaries
- **Each property entry in the database includes a margin of experimental error**
  - Determined on a case-by-case basis
  - This list is constantly expanding. The data is based on the outputs of 140+ independent experimental studies in literature.

MSTDB-TP Expansion Efforts

- **Outdated figures should no longer be referenced**
- **Still flowing roadmap guidance!**





Mcmurray, Jake W., et al. Roadmap for thermal property measurements of Molten Salt Reactor systems. No. ORNL/SPR-2020/1865. Oak Ridge National Lab.(ORNL), Oak Ridge, TN (United States), 2021.

MSTDB-TP Expansion Efforts

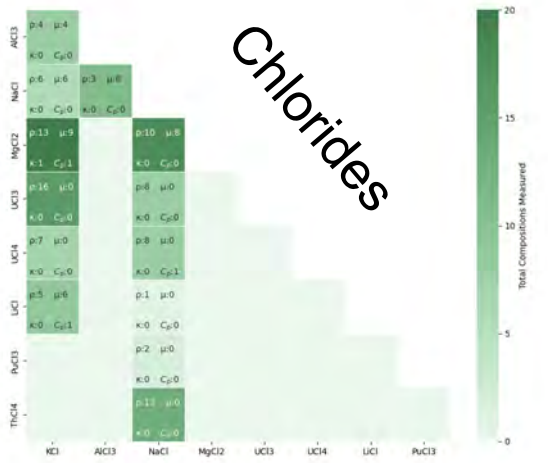
Available @ mstdb.ornl.gov

- **MSTDB-TP has undergone 2 major expansion efforts:**
  - 1.0 to 2.0 (68 entries to 273 entries)
  - 2.0 to 2.1 (273 entries to 448 entries)
- **These expansions incorporate replacements of old datasets as well**
  - E.g. recent literature has suggested UCl3 and relevant mixtures has a lower thermal expansion coefficient than previously understood
- **MSTDB-TP is being expanded for later releases**
  - This includes new pseudo-binary and higher order system data that exist in literature and need evaluated
  - MSTDB-TP will also include new data of new systems as it is published
- **MSTDB-TP is intending on including surface tension data in the future**
  - There is a significant body of literature already evaluated and tabulated

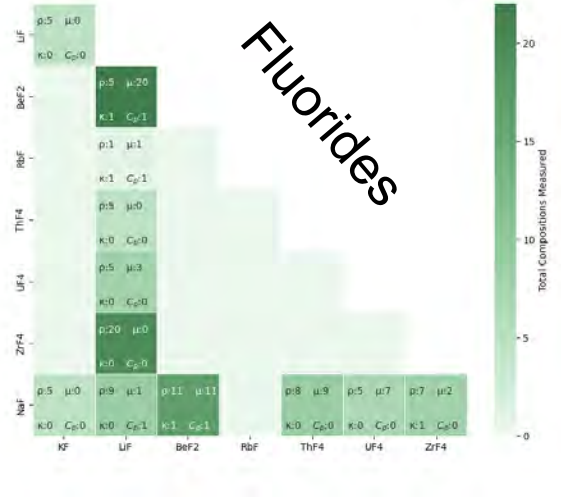
Pure:

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

Binary:



Living database



Ternary:

Salt	Measurements			
	ρ	μ	κ	c_p
KCl-LiCl-NaCl	4	0	0	0
LiCl-NaCl-AlCl3	10	10	0	0
LiF-BeF2-ThF4	3	2	0	0
LiF-BeF2-ZrF4	1	0	0	0
LiF-NaF-BeF2	1	1	0	0
LiF-NaF-KF	1	1	1	1
LiF-BeF2-UF4	36	36	0	0
NaF-BeF2-UF4	79	71	0	0
NaF-KF-BeF2	1	1	0	0
NaF-KF-MgCl2	1	0	0	0
NaF-KF-UF4	1	1	1	1
NaF-KF-ZrF4	1	1	0	0
NaF-LiF-BeF2	4	4	0	0
NaF-LiF-ZrF4	10	1	0	1
NaF-ZrF4-UF4	5	3	2	3
RbF-ZrF4-UF4	2	2	1	1

Quaternary:

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

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- **MSTDB-TP is intending on including surface tension data in the future**
  - There is a significant body of literature already evaluated and tabulated

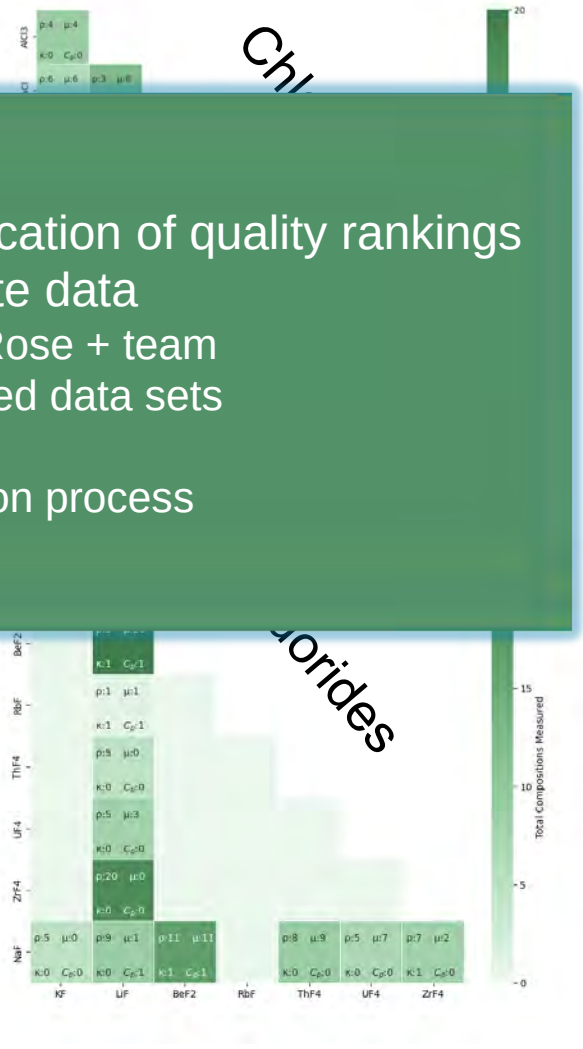
The MSR Campaign is funding the application of quality rankings to data in MSTDB-TP as well as duplicate data

- In collaboration with ANL – Melissa Rose + team
- Increased confidence in recommended data sets
- Better characterization of uncertainty
- Improved visibility about data selection process

Pure:

Salt	Measurements			
	ρ	μ	κ	c_p
AlCl3	1	1	0	1
BeCl2	1	0	0	0
BeF2	1	1	1	1
CaCl2	1	1	1	1
CaF2	1	1	1	1
NpF3	0	0	0	0
PuCl3	0	0	0	1
PuF3	0	0	0	1
SrCl2	1	1	1	0
SrF2	1	1	1	0
ThCl4	1	0	0	0
ThF4	1	0	0	0
UCl3	1	0	0	1
UCl4	1	0	0	0
UF3	0	0	0	1
UF4	1	1	0	1
ZrCl4	1	1	0	0
ZrF4	1	0	0	0

Binary:



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Salt	Measurements			
	ρ	μ	κ	c_p
KCl-LiCl-NaCl	4	0	0	0
LiCl-NaCl-AlCl3	10	10	0	0
LiF-BeF2-ThF4	3	2	0	0
LiF-BeF2-ZrF4	1	0	0	0
LiF-NaF-BeF2	1	1	0	0
LiF-NaF-KF	1	1	1	1
LiF-BeF2-UF4	36	36	0	0
NaF-BeF2-UF4	79	71	0	0
NaF-KF-BeF2	1	1	0	0
NaF-KF-MgCl2	1	0	0	0
NaF-KF-UF4	1	1	1	1
NaF-KF-ZrF4	1	1	0	0
NaF-LiF-BeF2	4	4	0	0
NaF-LiF-ZrF4	10	1	0	1
NaF-ZrF4-UF4	5	3	2	3
RbF-ZrF4-UF4	2	2	1	1

Quaternary:

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

Redlich-Kister Density Models

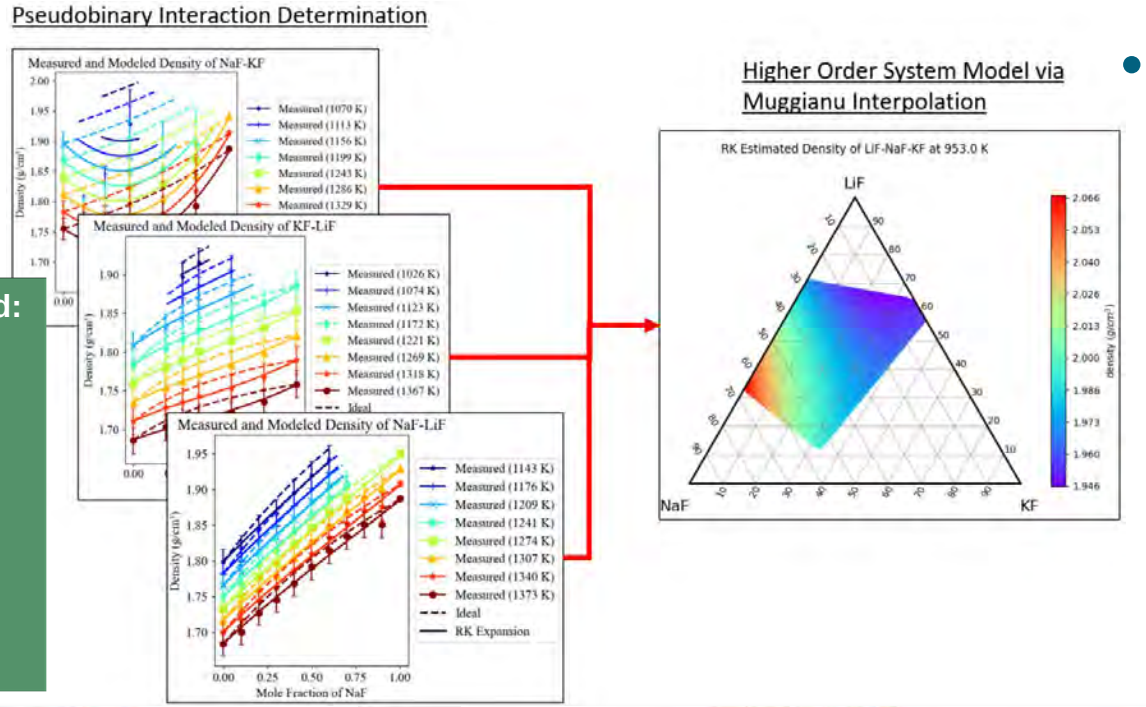
RK Parameters Generated:

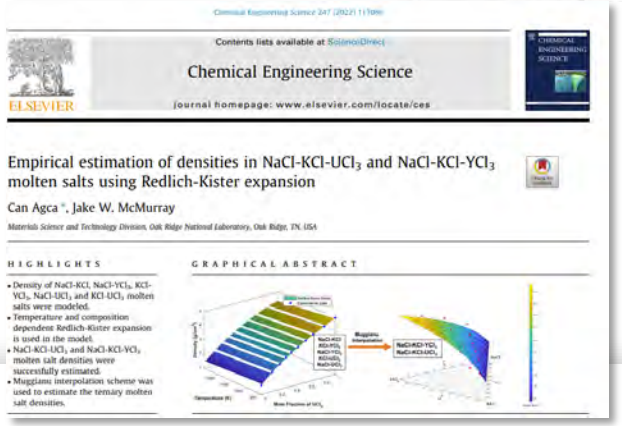
Fluorides

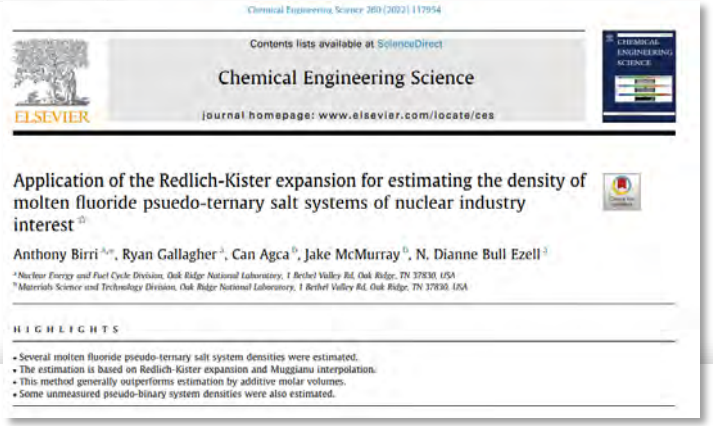
LiF-BeF2, LiF-KF, NaF-KF, NaF-LiF, NaF-ThF4, LiF-UF4, LiF-ZrF4, LiF-ThF4, NaF-ZrF4, NaF-UF4

Chlorides

LiCl-KCl, KCl-MgCl2, KCl-NaCl, KCl-UCl3, KCl-UCl4, NaCl-LiCl




Contents lists available at ScienceDirect
Chemical Engineering Science
journal homepage: www.elsevier.com/locate/ces
Empirical estimation of densities in NaCl-KCl-UCl_3 and NaCl-KCl-YCl_3 molten salts using Redlich-Kister expansion
Can Agca, Jake W. McMurray
HIGHLIGHTS
GRAPHICAL ABSTRACT


Contents lists available at ScienceDirect
Chemical Engineering Science
journal homepage: www.elsevier.com/locate/ces
Application of the Redlich-Kister expansion for estimating the density of molten fluoride psuedo-ternary salt systems of nuclear industry interest
Anthony Birri, Ryan Gallagher, Can Agca, Jake McMurray, N. Dianne Bull Ezell
HIGHLIGHTS
- Several molten fluoride pseudo-ternary salt system densities were estimated.
- The estimation is based on Redlich-Kister expansion and Muggianu interpolation.
- This method generally outperforms estimation by additive molar volumes.
- Some unmeasured pseudo-binary system densities were also estimated.

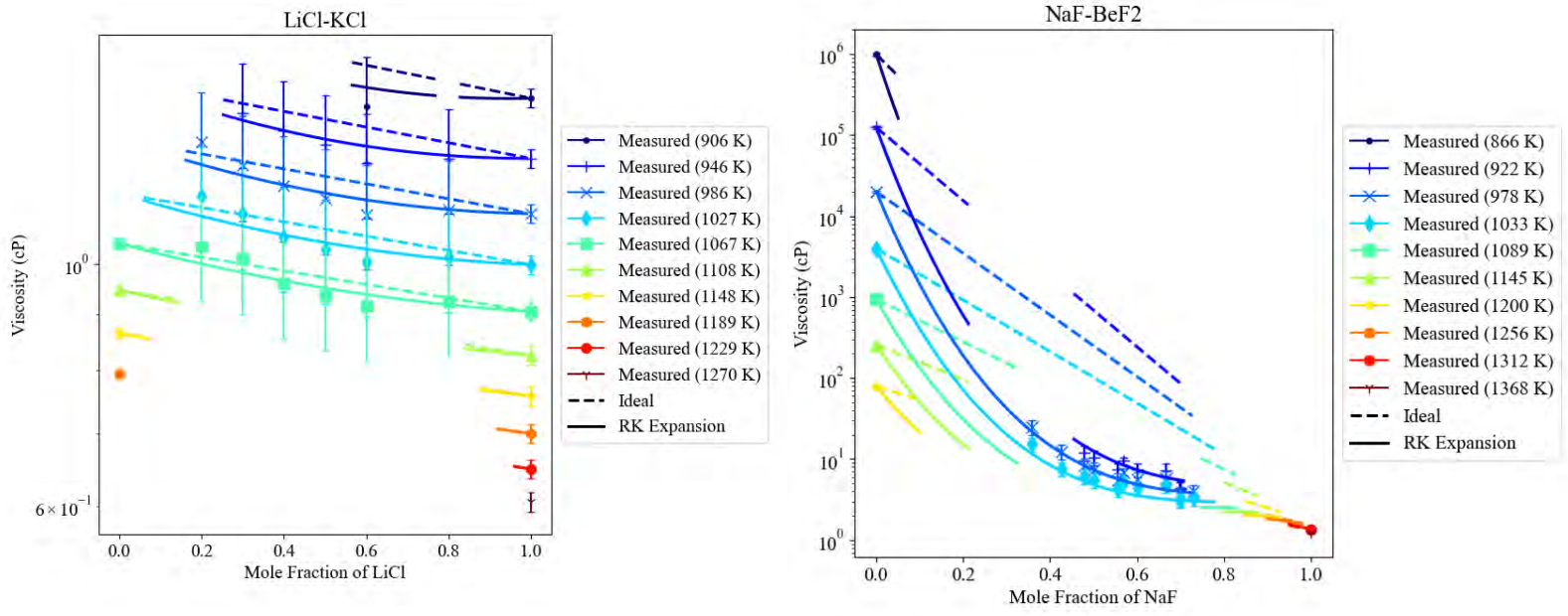
- **Motivation: We can only make measurements across the national laboratories so fast**
  - Limited time and funding
  - There are countless possible pseudo-ternary+ systems which may be of interest
  - Therefore, implementing Redlich-Kister framework with Muggianu extrapolation need estimation techniques to predict thermophysical properties of higher-order systems

More Information Available in FY23 Status Milestone Report – Available this summer

Ongoing Effort: Viscosity Estimation

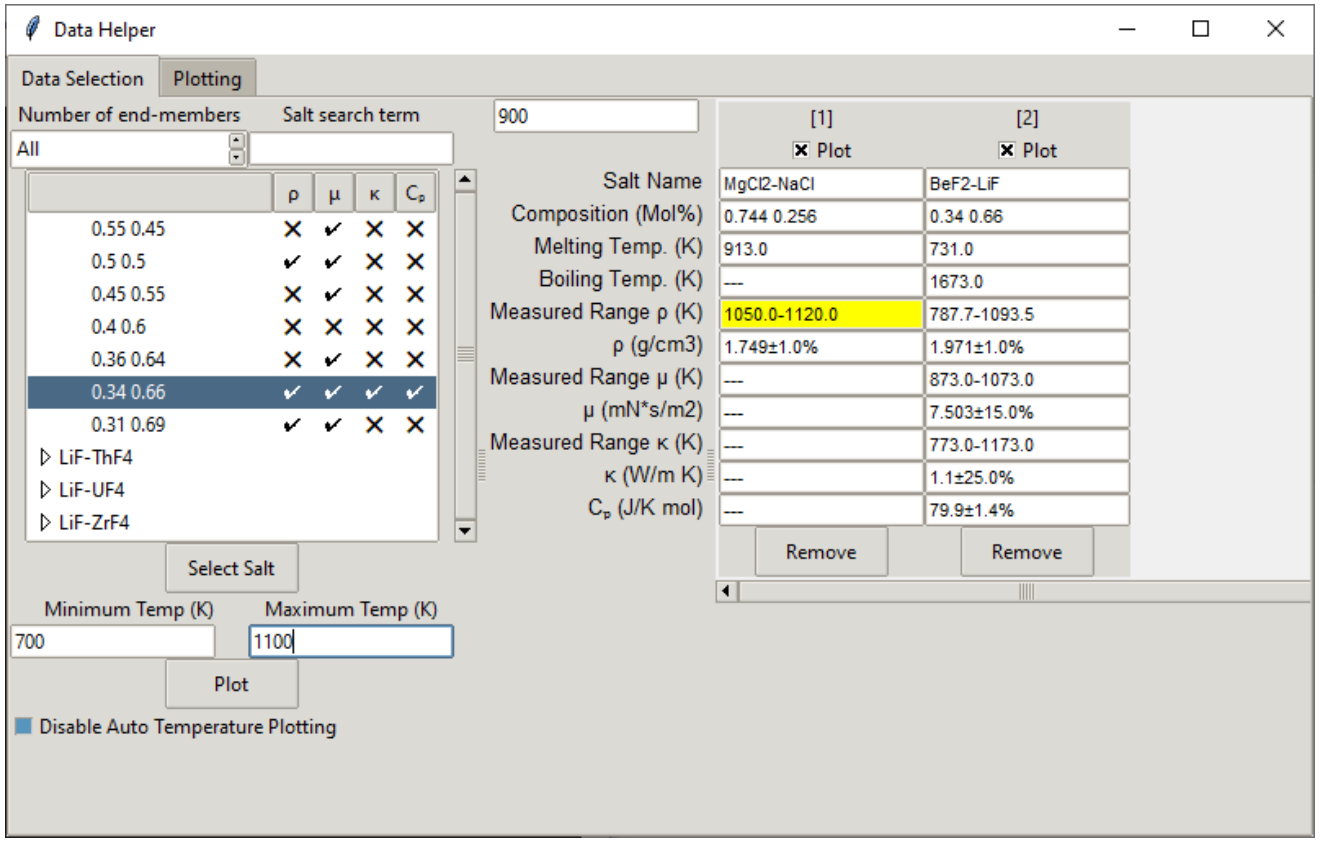
- **Viscosity Estimation is proving to be more challenging than density**
  - Multiple manners by which one may model ideal or non-ideal terms
    - Ideal mixing: Gambill method, Grunburg-Nissan rule, Katti-Chaudhri rule
    - Non-Ideal terms: RK, modified Grunburg-Nissan
- We are investigating ALL possible methods and different orders of fit to find a consistent, generalizable method
- The ultimate goal is to validate extrapolative capabilities with higher-order systems

Results of some tests from Grunburg-Nissan
Ideal mixing with RK interaction terms



User/Modeler Accessibility through GUI or API

- **MSTDB-TP is a large, difficult to navigate .csv file**
- **Saline is the MSTDB-TP API**
  - Provides a stable C++ interface for obtaining supported properties (density, viscosity, heat capacity, and thermal conductivity)
  - Designed for integration with other NEAMS codes
- **The MSTDB-TP GUI allows for easier navigation and visualization of the data**



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The authors would like to thank **Ted Besmann** for guidance on MSTDB-TP development decisions.

Thank you

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