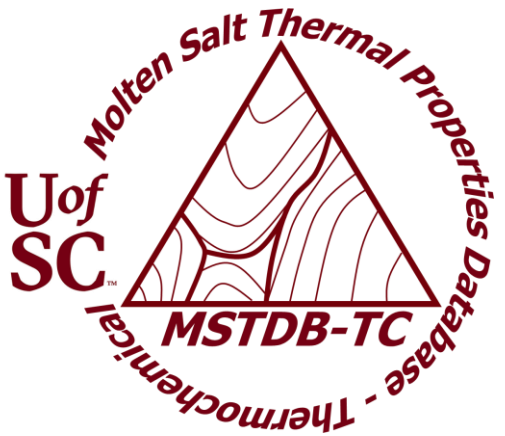
General Atomics SmartState Center for Transformational Nuclear Technologies

Molten Salt Thermal Properties Database-Thermochemical (*MSTDB-TC)*

T. M. Besmann
University of South Carolina

UNIVERSITY OF South Carolina



Some of Our Contributors and Collaborators

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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

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Base Salt Systems From Current Program Roadmap

ORNL/SPR-2020/1865

Roadmap for thermal property measurements of Molten Salt Reactor systems

Thermal spectrum: Fluoride systems

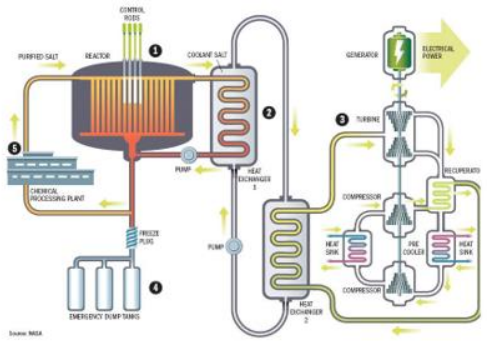
- $LiF\text{-}BeF_2\text{-}UF_3\text{-}UF_4\text{-}ZrF_4$
- $NaF\text{-}BeF_2\text{-}UF_3\text{-}UF_4\text{-}ThF_4$
- $LiF\text{-}NaF\text{-}ThF_4$
- $NaF\text{-}BeF_2\text{-}UF_3\text{-}UF_4\text{-}ThF_4$

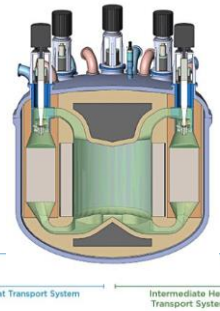
Solely heat transfer medium

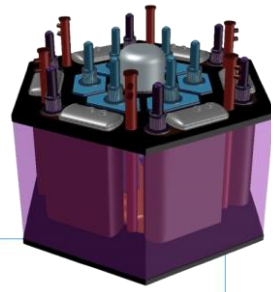
- $NaF\text{-}BeF_2$
- $LiF\text{-}BeF_2$
- $LiCl\text{-}NaCl\text{-}MgCl_2$

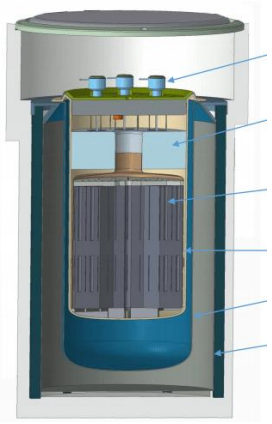
Fast spectrum: Chloride systems

- $NaCl\text{-}MgCl_2\text{-}UCl_3\text{-}UCl_4\text{-}PuCl_3$,
- $NaCl\text{-}ZrCl_4\text{-}UCl_3\text{-}UCl_4\text{-}PuCl_3$,
- $NaCl\text{-}AlCl_3\text{-}UCl_3\text{-}UCl_4\text{-}PuCl_3$,
- $NaCl\text{-}KCl\text{-}MgCl_2\text{-}UCl_3\text{-}UCl_4\text{-}PuCl_3$,
- $NaCl\text{-}KCl\text{-}ZrCl_4\text{-}UCl_3\text{-}UCl_4\text{-}PuCl_3$,
- $NaCl\text{-}KCl\text{-}AlCl_3\text{-}UCl_3\text{-}UCl_4\text{-}PuCl_3$,
- $NaCl\text{-}ThCl_4\text{-}PuCl_3$









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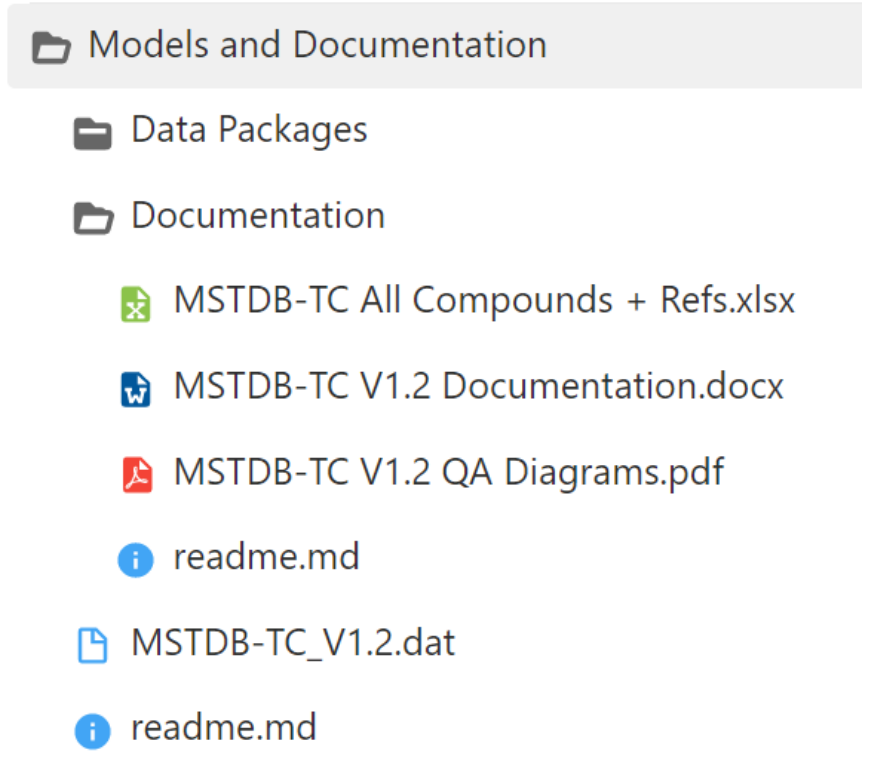
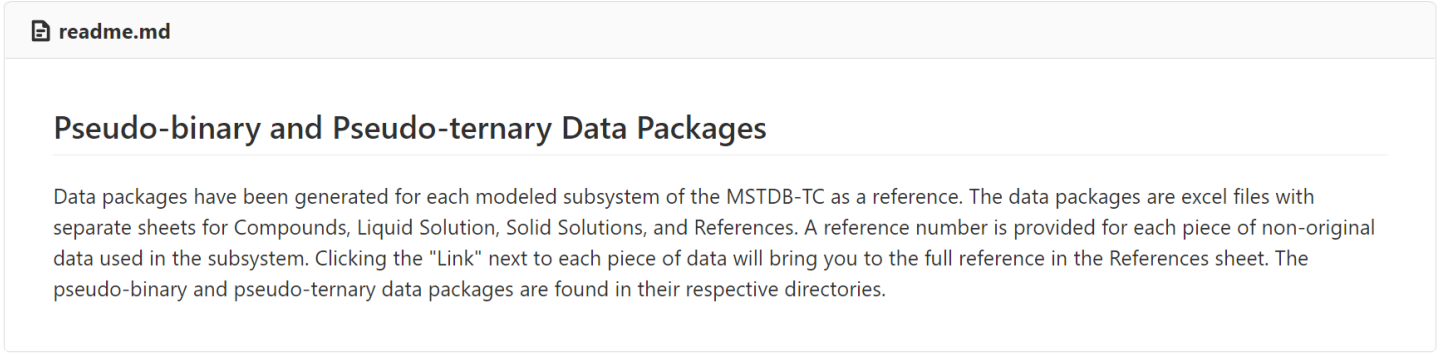
Thermodynamic Modeling Requires an Accurate, Consistent and Extensive Gibbs Energy Database

- Database consists of Gibbs energy relations for each phase and gas species
- Gibbs energy relations for (stoichiometric) compounds are obtained from
  - Directly from accurate reported values
  - Assessment of reported data and/or measurements
- Solid and liquid solutions need to be represented by models that provide Gibbs energy relations at specific temperature, pressure, and composition (gas typically an ideal solution)
  - Directly from accurate reported values consistent with basic database phase values, or
  - Reassessment of reported models using new data and consistent base values, or
  - Full assessment from reported values/new measurements using consistent base values
- Resource is the *Molten Salt Thermal Properties Database – Thermochemical* (*MSTDB-TC)*

MSTDB-TC - Structure

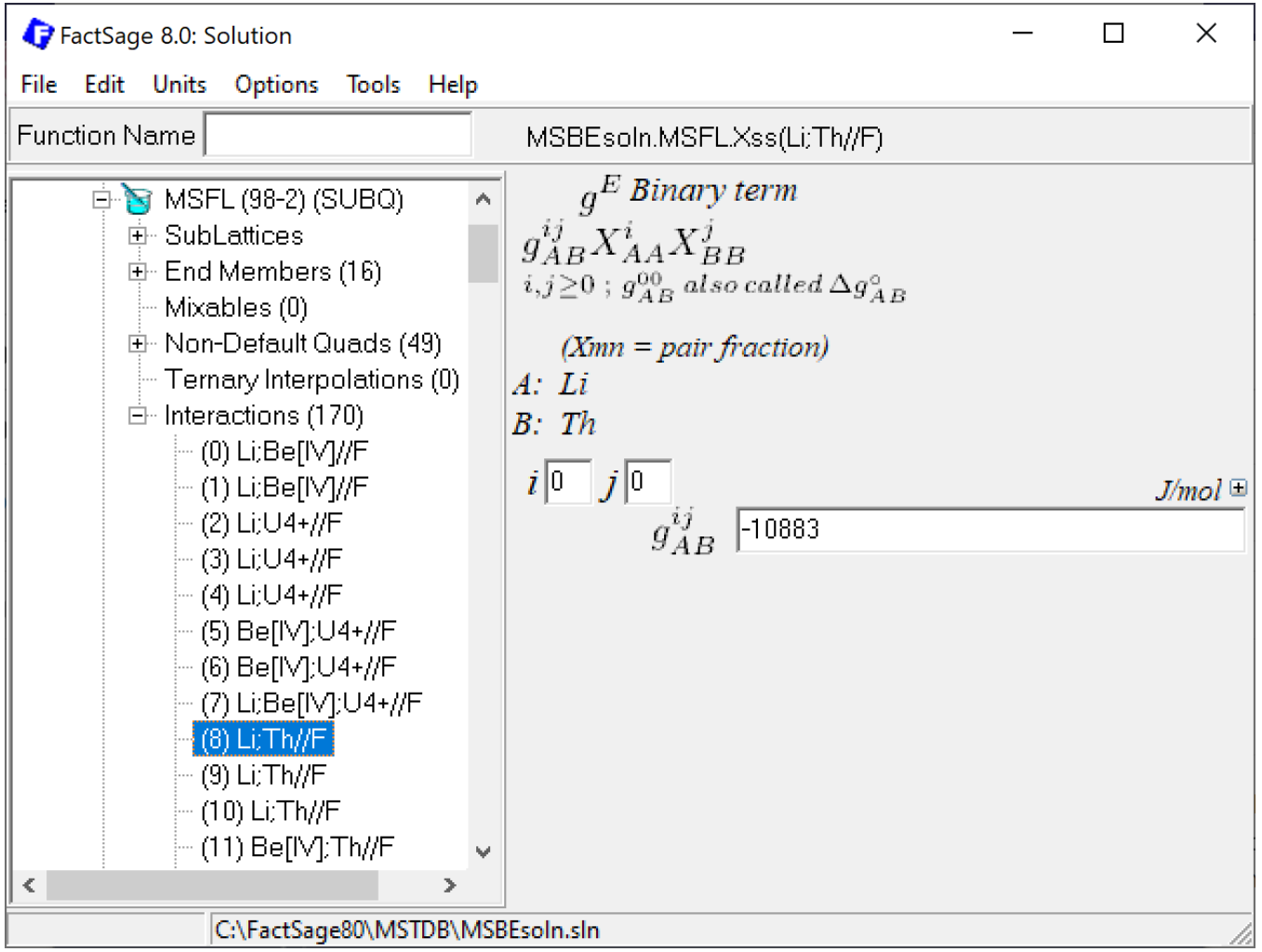
- Hosted by Oak Ridge National Lab (ORNL) on Code.ornl GitLab repository as a series of files and directories.
- Download entire database, or individual files
- Native GitLab Readme documentation for each directory





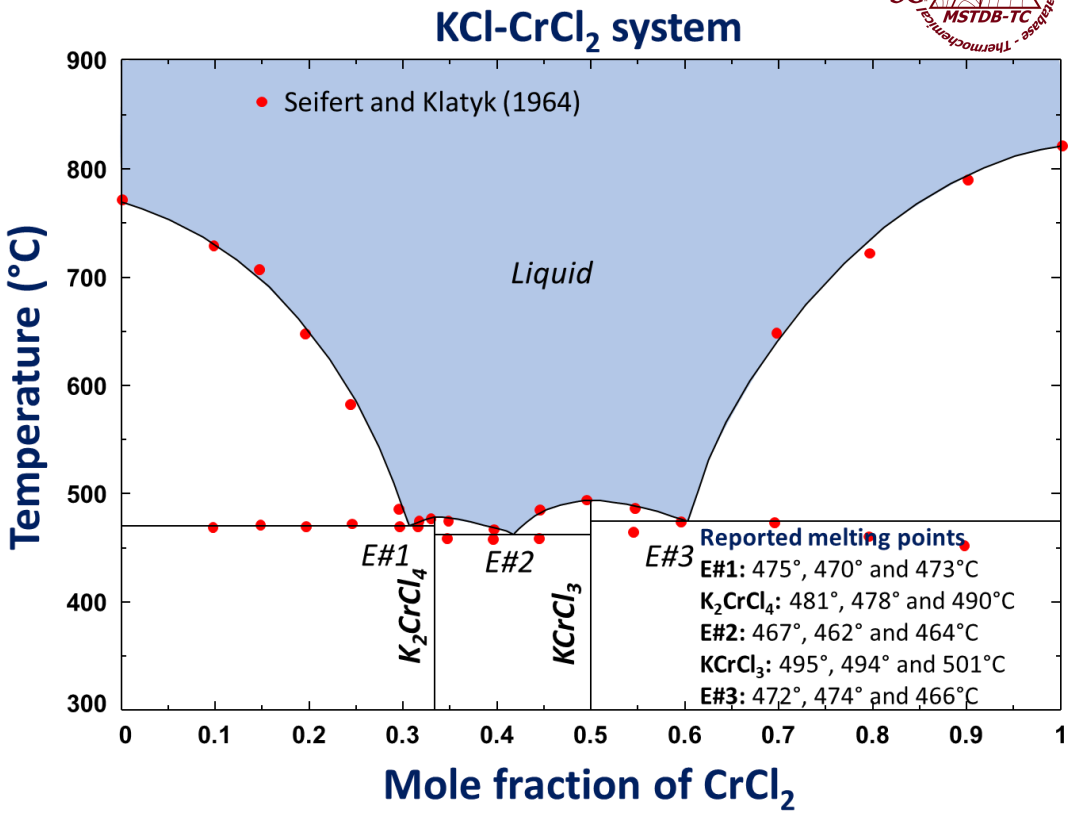
MSTDB-TC - Modeling

- Performed following the CALPHAD method
- Liquid (melt) solutions use the Modified Quasi-chemical Model in the Quadruplet Approximation (MQMQA)
- Solid solutions modeled using the single sublattice polynomial model or Compound Energy Formalism (CEF)



MSTDB-TC – Assessments Fit Model Parameter to Reproduce Phase Equilibria and Thermodynamc Properties

- Published models
  - If compatible, input as-published
- Reassessments
  - Affected by changes to other systems
  - Different models or pure compound values
  - New data, errant values, etc.
- Original assessments
  - Novel systems
  - Use of multi-coordination endmembers



MSTDB-TC Format is Open and Directly Usable by Equilibrium Calculation Codes

- *MSTDB-TC* Follows the FactSage ASC II Format (.dat)
- Database provides
  - Thermodynamic functions readable by FactSage™ and open-source code Thermochimica
  - Pseudo-binary and higher order system data
    - Reference values from literature with sources
    - Original measurements including uncertainties
    - Details of function fitting and uncertainties
- All systems validated via reproduction of accepted phase equilibria
  - Verified via examination of all systems by third-party (ORNL)

```
System U-F-Li
    3    2    2    3   12
 U                        F                        Li
   238.02891000             18.99840320              6.94100000
   6   1   2   3   4   5   6
   6   1   2   3   4   5   6
 gas_ideal
 IDMX
 LiF
   1  1    0.0    1.0    1.0
  6000.0000     -351581.57      37.443358     -35.397917     -.93533200E-03
 0.27571767E-07 0.00000000
UF4
   1  1    1.0    4.0    0.0
  6000.0000     -1639992.8      343.21185     -103.82600     -.47745000E-02
 0.24183333E-06  510660.00
LIQUsoln
 SUBG
  2.40000
   2   3
 Li//F
   1  1    0.0    1.0    1.0
  2500.0000     -617790.20      386.90980     -64.182999     0.00000000
 0.00000000     0.00000000
  1.00000      1.00000     0.000000     0.000000     0.000000
 U//F
   1  1    1.0    4.0    0.0
  2500.0000     -1966756.7      1054.9383     -174.74000     0.00000000
 0.00000000     0.00000000
  1.00000      4.00000     0.000000     0.000000     0.000000
   2   1
 Li                       U
 F
  1.00000      4.00000
   1   2
  1.00000
   1
   1   2
   1   1
   1   1   3   3  6.0000000      6.0000000      6.0000000      6.0000000
   2   2   3   3  6.0000000      6.0000000      1.5000000      1.5000000
   1   2   3   3  2.0000000      6.0000000      1.7142857      1.7142857
   3
 G   1   2   3   3   0   0   0   0
 0.00000000       1.00 0.00000000       1.00 0.00000000       1.00
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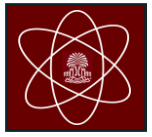

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MSTDB-TC V1.2 Content

- 94 Pseudo-binary systems
- 37 Pseudo-ternary systems
- 42 Solid Solutions
- 201 Stoichiometric compounds

- Fluorides:
  - 51 pseudo-binary
  - 26 pseudo-ternary
  - 26 solid solutions

- Chlorides:
  - 43 pseudo-binary
  - 11 pseudo-ternary
  - 16 solid solutions

MSTDB-TC Fluoride Systems Content: Be-Ca-Ce-Cs-K-La-Li-Na-Ni-Nd-Pu-Rb-Th-U-F

Pseudo-ternary and higher order systems

- BeF2-LiF-NaF
- BeF2-LiF-PuF3
- BeF2-LiF-ThF4
- BeF2-LiF-UF4
- BeF2-NaF-PuF3
- BeF2-NaF-ThF4
- BeF2-NaF-UF4
- BeF2-ThF4-UF4
- CaF2-KF-NaF
- CaF2-LaF3-LiF
- CaF2-LaF3-NaF
- CaF2-LiF-KF
- CaF2-LiF-ThF4
- CeF3-LiF-ThF4
- CsF-LaF3-LiF
- CsF-LiF-KF
- CsF-LiF-PuF3
- LaF3-LiF-NaF
- LiF-KF-NaF
- LiF-KF-RbF
- LiF-NaF-CeF3
- LiF-NaF-PuF3
- LiF-NaF-RbF
- LiF-NaF-ThF4
- LiF-NaF-UF4
- LiF-PuF3-ThF4
- LiF-PuF3-UF4
- LiF-ThF4-CaF2
- LiF-NaF-BeF2-ThF4-PuF3-UF4
- LiF-NaF-BeF2-KF-PuF3-UF4
- LiF-NaF-KF-CsF-ThF4-PuF3

Matrix of pseudo-binary systems

	LiF	NaF	BeF_2	KF	RbF	CaF_2	ZrF_4	ThF_4	PuF_3	UF_4	UF_3	CsF	CeF_3	LaF_3	SrF_2	MgF_2	NdF_3	FeF_2
NaF	✓																	
BeF_2	✓	✓																
KF	✓	✓	✓															
RbF	✓	✓		✓														
CaF_2	✓	✓	✓	✓														
ZrF_4	✓		✓															
ThF_4	✓	✓	✓			✓												
PuF_3	✓	✓	✓	✓	✓			✓										
UF_4	✓	✓	✓	✓			✓	✓	✓									
UF_3	✓	✓								✓								
CsF	✓	✓		✓	✓			✓	✓	✓	✓							
CeF_3	✓	✓						✓										
LaF_3	✓	✓		✓	✓	✓			✓			✓						
SrF_2	✓	✓		✓		✓												
MgF_2	✓	✓		✓		✓									✓			
NdF_3	✓																	
FeF_2		✓																
NiF_2	✓	✓		✓														

✓ In *MSTDB-TC*
✓ Data Published

MSTDB-TC Chloride Systems Content: Al-Ca-Ce-Cs-Fe-K-Li-Mg-Na-Ni-Pu-Rb-U-Cl

Pseudo-ternary and higher order systems

- CeCl3-KCl-LiCl
- CeCl3-KCl-MgCl2
- CeCl3-KCl-NaCl
- CeCl3-LiCl-MgCl2
- KCl-LiCl-UCl3
- LiCl-NaCl-MgCl2-KCl-PuCl3-UCl3
- LiCl-NaCl-MgCl2-KCl-CeCl3

Matrix of pseudo-binary systems

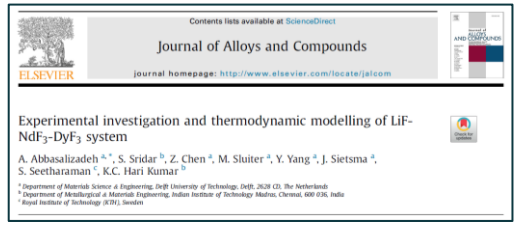
	LiCl	NaCl	$MgCl_2$	KCl	RbCl	$CaCl_2$	CsCl	$PuCl_3$	UCl_3	$ZnCl_2$	$MnCl_2$	$FeCl_2$	$CoCl_2$	$NiCl_2$	$SrCl_2$	$CeCl_3$	$AlCl_3$
NaCl	✓																
$MgCl_2$	✓	✓															
KCl	✓	✓	✓														
RbCl	✓	✓	✓	✓													
$CaCl_2$	✓	✓	✓	✓	✓												
CsCl	✓	✓	✓	✓	✓	✓											
$PuCl_3$		✓	✓	✓	✓		✓										
UCl_3	✓	✓	✓	✓				✓									
$ZnCl_2$		✓	✓	✓		✓											
$MnCl_2$		✓	✓	✓		✓				✓							
$FeCl_2$		✓	✓	✓		✓				✓	✓						
$CoCl_2$		✓	✓	✓		✓				✓	✓	✓					
$NiCl_2$		✓	✓	✓		✓				✓	✓	✓	✓				
$SrCl_2$	✓	✓	✓	✓		✓											
$CeCl_3$	✓	✓	✓	✓		✓											
$AlCl_3$	✓	✓	✓	✓													
$FeCl_3$		✓		✓								✓					

✓ In *MSTDB-TC*
✓ Data Published

MSTDB-TC Sources Vary From Values Directly Extracted From Publications to Derived From Original Measurements

All values traceable to original sources via provided data packages

- Pure substance, single cation phase values from tabulated sources, e.g., NIST, SGTE via FactSage™
- Melt, solid solution, or complex compound models and values/parameters are
  - Obtained as is from published papers/reports
  - Determined in assessments/reassessments using values from published papers/reports
  - Computed for compounds obtained using *ab initio* modeling & used in assessments
  - Obtained using measurements for assessments from original experimental efforts


Contents lists available at ScienceDirect

Journal of Alloys and Compounds

journal homepage: http://www.elsevier.com/locate/jalcom

Experimental investigation and thermodynamic modelling of LiF-NdF_3-DyF_3 system

A. Abbasalizadeh [a,*], S. Sridar [b], Z. Chen [a], M. Sluiter [a], Y. Yang [a], J. Sietsma [a], S. Seetharaman [c], K.C. Hari Kumar [b]

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[b] Department of Metallurgical & Materials Engineering, Indian Institute of Technology Madras, Chennai, 600 036, India
[c] Royal Institute of Technology (KTH), Sweden

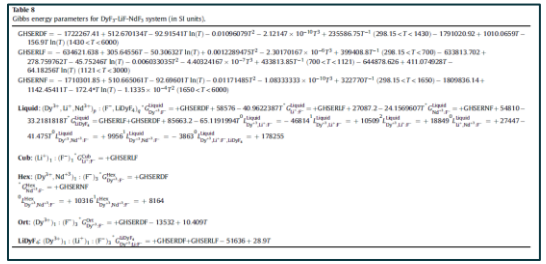
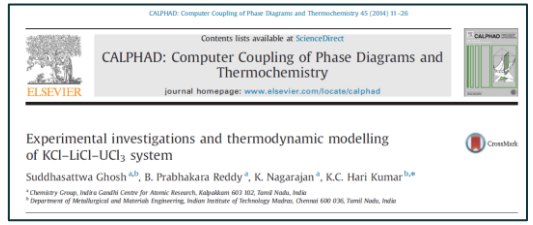


Table 8
Gibbs energy parameters for DyF_3-LiF-NdF_3 system (in SI units).


CALPHAD: Computer Coupling of Phase Diagrams and Thermochemistry 45 (2014) 11–26

Contents lists available at ScienceDirect

CALPHAD: Computer Coupling of Phase Diagrams and Thermochemistry

journal homepage: www.elsevier.com/locate/calphad

Experimental investigations and thermodynamic modelling of KCl–LiCl–UCl_3 system

Suddhasattwa Ghosh [a,b], B. Prabhakara Reddy [a], K. Nagarajan [a], K.C. Hari Kumar [b,*]

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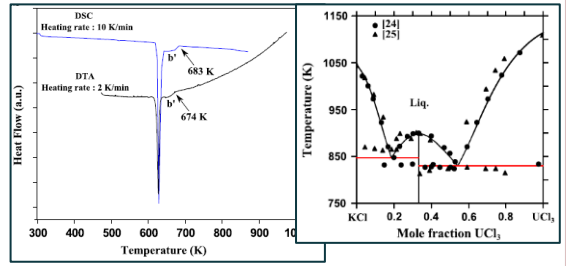
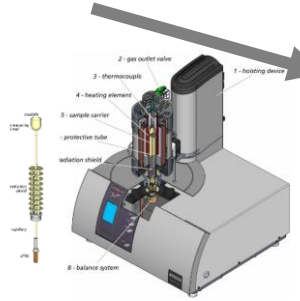
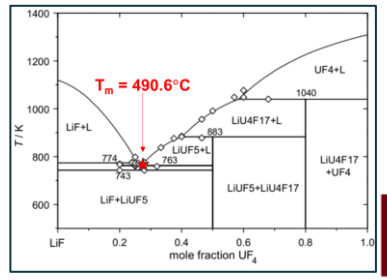
[b] Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, Chennai 600 036, Tamil Nadu, India

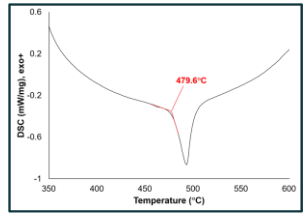


DFT

	H°0K (eV)	H°0K (J/mol)
K_2UF_6	-3.643	-3163464.3
K_3UF_7	-3.523	-3739095.7
$K_7U_6F_{31}$	-	
KU_2F_9	-3.858	-4466884.5







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Linked Data Packages for All Included Values

- Excel files for each modeled pseudo-binary and –ternary system:
  - Pure compounds
  - Liquid solutions
  - Solid solutions
  - Linked references
  - Reassessed and Original values

	A	B	C	D	E	F	G
1	Pseudo-binary Liquid Interaction Parameters						
2	Species A	Species B	i	j	Ref. #	Ref Link	Comments
3	LiF	KF	0	0	2	Link	Changed to (-7200 +4.8*T -0.0014*T^2)
4	LiF	KF	1	0	2	Link	Changed to (-1200)
5	NaF	KF	0	0	2	Link	
6	NaF	KF	1	0	2	Link	
7	LiF	NaF	0	0	7	Link	Changed to (-2639.4 +0.921*T)
8	LiF	NaF	1	0	7	Link	Set to 0
9	LiF	NaF	0	1	7	Link	Changed to (50)

	A	B	C	D	E	F	G	H
1	Ref. Number	Authors	Year	Title	Publication	Issue/Chapter	Pages	ORNL Doc #
2	1	E. Capelli, O. Benes, R.J.M Konings	2014	Thermodynamic assessment of the LiF-NaF-BeF2-ThF4-UF4 system	Journal of Nuclear Materials	449	111-121	
3	2	O. Benes, R.J.M Konings	2008	Thermodynamic evaluation of the MF-LaF3 (M = Li, Na, K, Rb, Cs) systems	Calphad-Computer Coupling of Phase Diagrams and Thermochemistry	32	121-128	
4	3	O. Benes, R.J.M Konings	2008	Actinide burner fuel: Potential compositions based on the thermodynamic evaluation of MF-PuF3 (M = Li, Na, K, Rb, Cs) and LaF3-PuF3 systems	Journal of Nuclear Materials	377	449-457	

Testing for Reproducibility With Respect to Published Diagrams

- Each release version of the *MSTDB-TC* undergoes an ORNL evaluation
- Primary criteria is reproduction of modeled phase diagrams.
- *MSTDB-TC* computed diagrams provided side-by-side with published versions
  - Calculated phase diagram for all modeled systems
  - Compared against published diagrams
  - Notes section for discussion of selected systems
  - Provided in pdf with *MSTDB-TC* documentation

31: CsF-ThF4

Fig. 31a - Calculation saved in C:\FactSage80\MSTDB\PD Macro\BMPs\

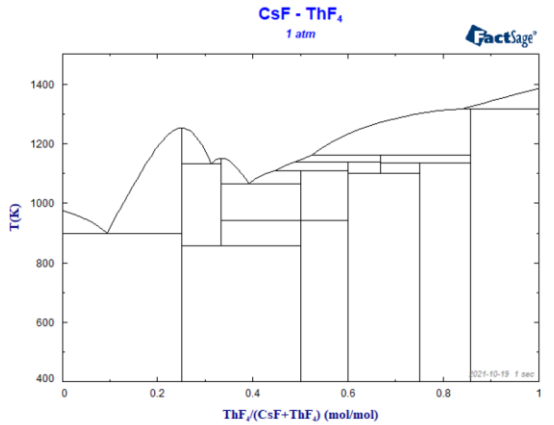
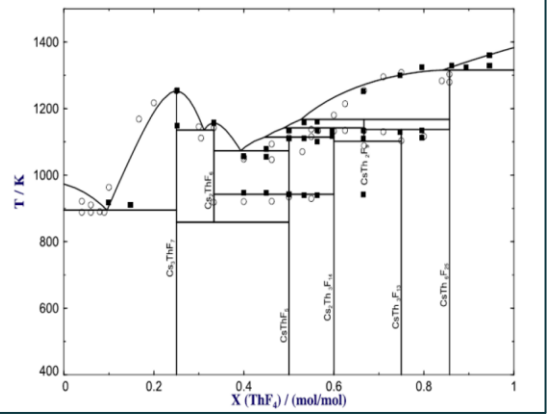


Fig. 31b - Published figure from Ref[9] saved in C:\FactSage80\MSTDB\PD_Macro\Lit
Please see Excel data package for this system for additional information.



103: LiF-NaF-PuF3

Fig. 103a - Calculation saved in C:\FactSage80\MSTDB\PD Macro\BMPs\

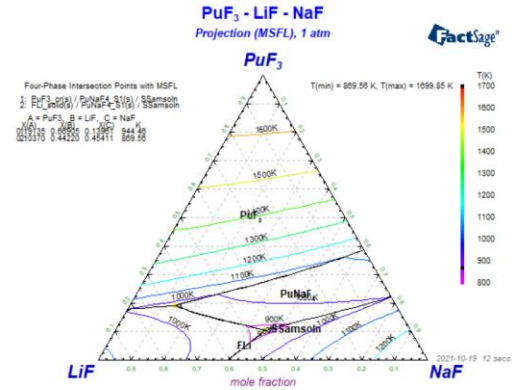
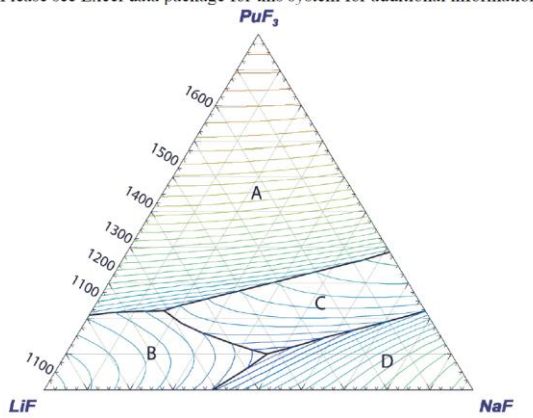


Fig. 103b - Published figure from Ref[3] saved in C:\FactSage80\MSTDB\PD_Macro\Lit
Please see Excel data package for this system for additional information.

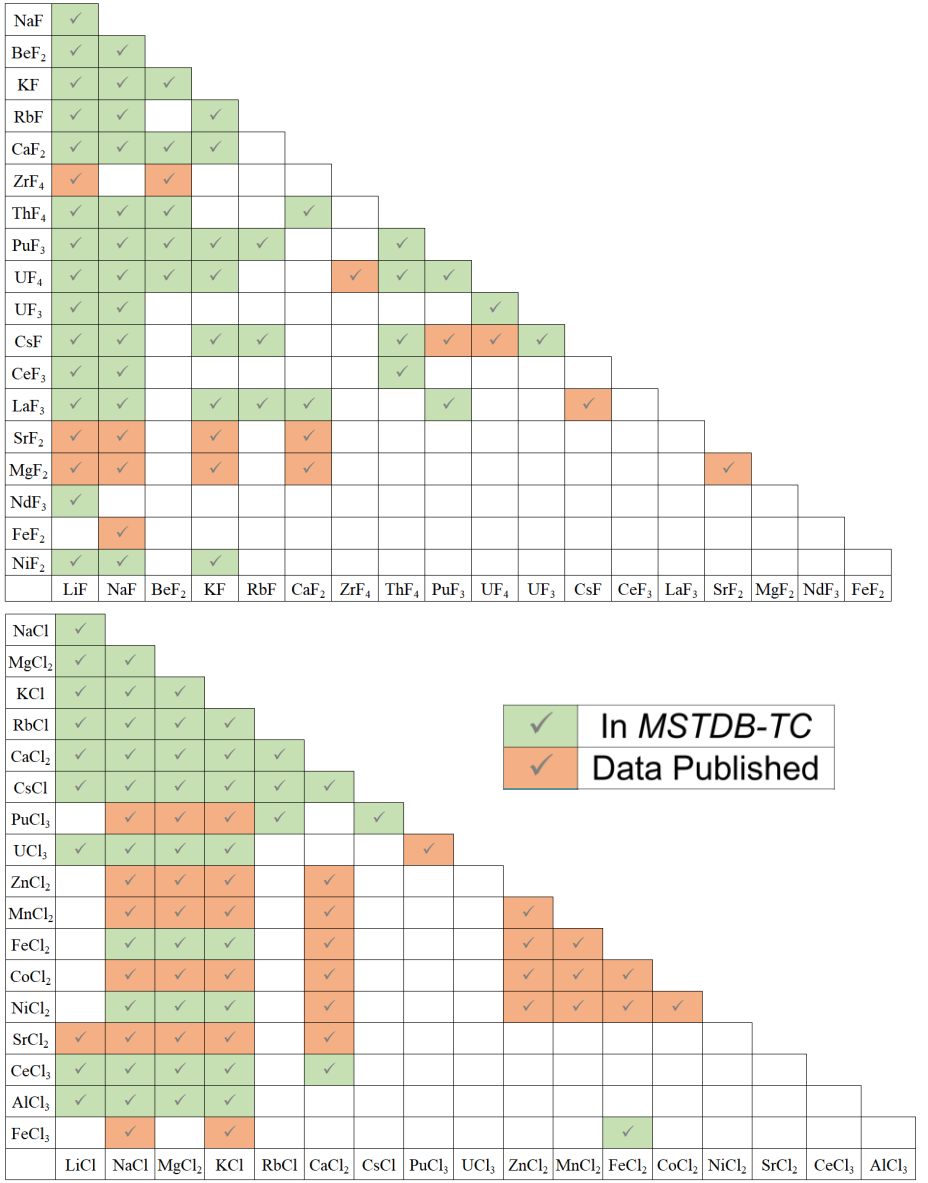


MSTDB-TC V1.2 Public Release

- First public version has been completed, tested, and made available at https://code.ornl.gov/neams/mstdb/
- Obtain cost-free after registering an ORNL XCAMS account and access approval
  - Create an account at https://xcams.ornl.gov
  - Email MSTDB@ornl.gov with subject 'MSTDB Access Request' and
    - Your XCAMS ID
    - A brief summary of the purpose of your access
  - You will receive an email from code.ornl.gov indicating your *MSTDB-TC* access has been granted and a link to the project page
- Permits access to *MSTDB-TP* as well

MSTDB-TC Future Updates

- Additional system assessments in-progress
  - Published models not yet added
  - Corrosion products (Fe, Ni, Cr)
  - Multi-coordination systems
  - Systems key for safety analysis (Cs, I…)
- Versions will be posted every few months with additional assessments/reassessments
  - New added systems
  - Revisions based on new information



General Atomics Center Researchers and Students

➢ *We are looking for new post-docs to join us!* ➢

General Atomics SmartState Center for Transformational Nuclear Technologies

U of SC South Carolina

OAK RIDGE National Laboratory

Molten Salt Thermal Properties Database – Thermophysical (MSTDB-TP)

Jake McMurray, Can Agca,

Shane Henderson, Robert Lefebvre

Tony Birri, and Dianne Ezell

Oak Ridge National Laboratory

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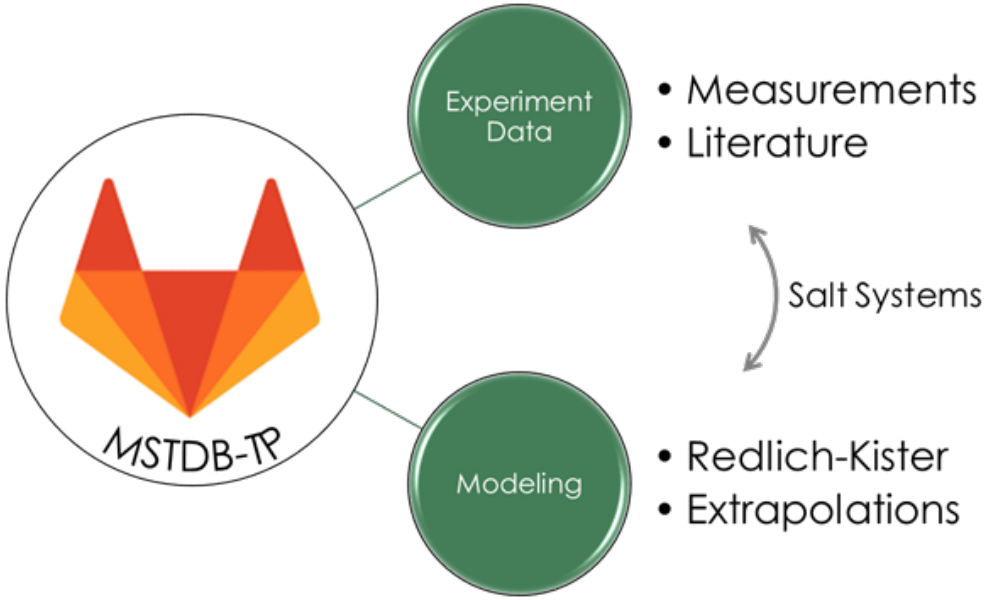
U.S. DEPARTMENT OF ENERGY

Vision/Mission



- The Molten Salt Thermal Properties Database (MSTDB) is a database of models and model parameters that will represent salt solution thermal property behavior as a function of temperature and composition
  - **T**hermo**c**hemical division is designated MSTDB-TC
  - **T**hermophysical **p**roperties division is designated MSTDB-TP

Molten Salt Thermophysical Database 1.0

- **MSTDB-TP Version 1.0 finalized (open access soon to be available)**

- Type of data (along with references and uncertainty)
  - Melting temperature
  - Boiling temperature
  - Density
  - Viscosity
  - Thermal Conductivity
  - Heat capacity

- 62 entries currently: 27 pure, 8 binaries, 10 ternaries & 5 quaternaries

Molten Salt Thermophysical Database 1.0

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  - Density
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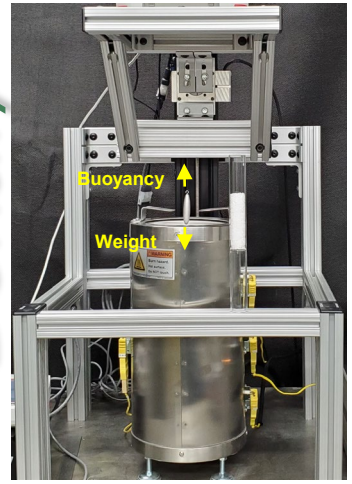
  - Thermal Conductivity
  - Heat capacity

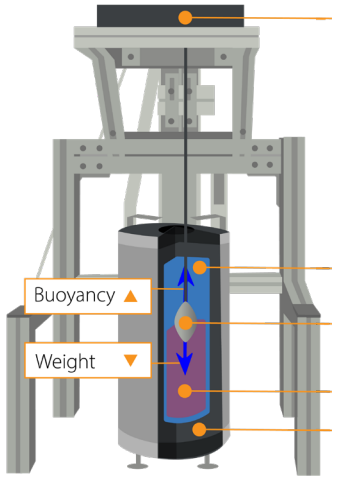
- 62 entries currently: 27 pure, 8 binaries, 10 ternaries & 5 quaternaries
  - Thermal conductivity needs data through either experiments or theoretical studies

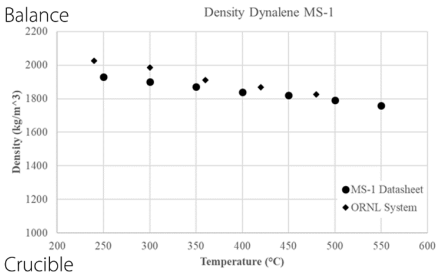
Thermophysical Characterizations

Density

Archimedes Bob Density Measurement Apparatus

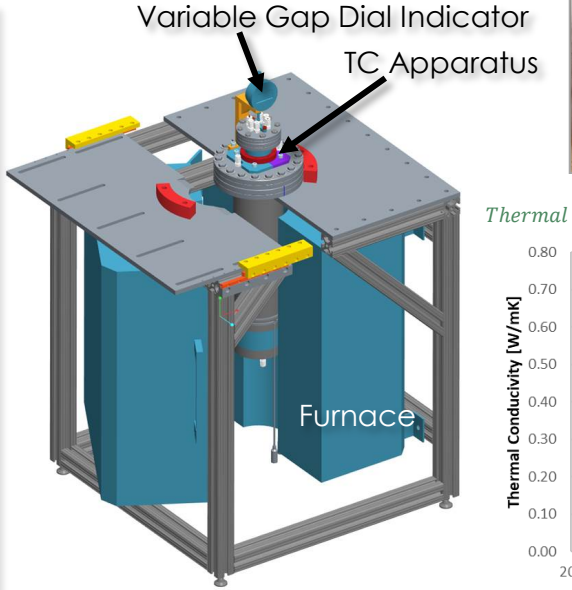


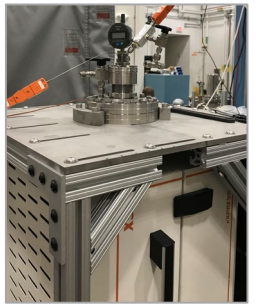




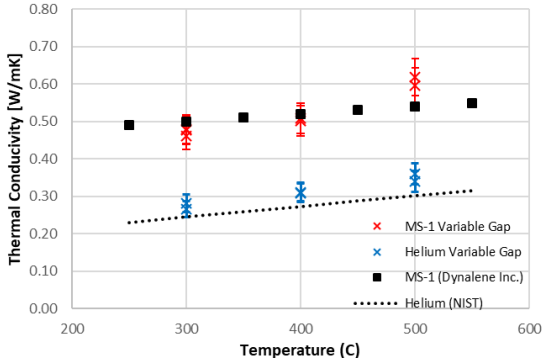
Alternate methods:
Optical dilatometry
X-ray dilatometry

Thermal Conductivity

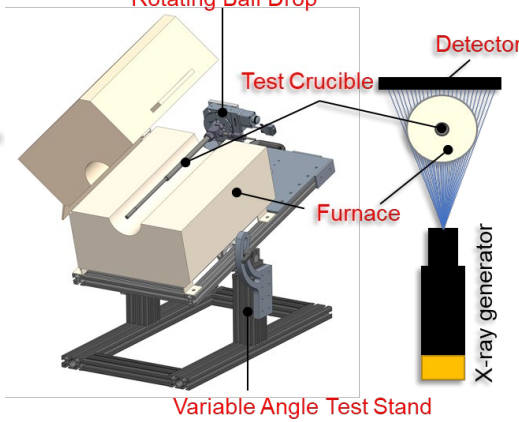


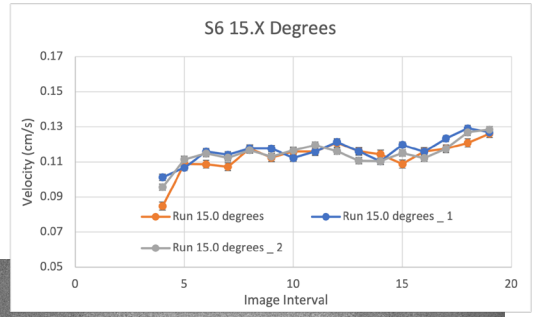


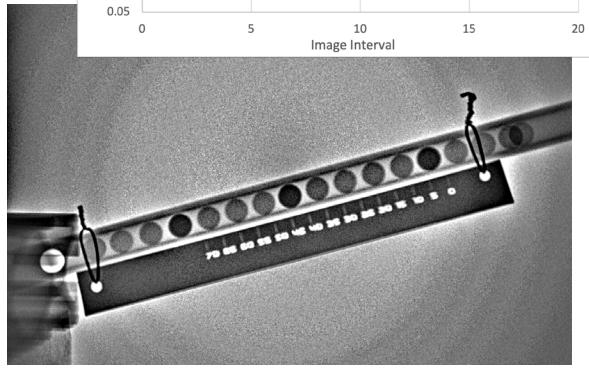
$$\text{Thermal Resistance} = \frac{\text{Change in temperature across gap}}{\text{heat flux}}$$



Viscosity

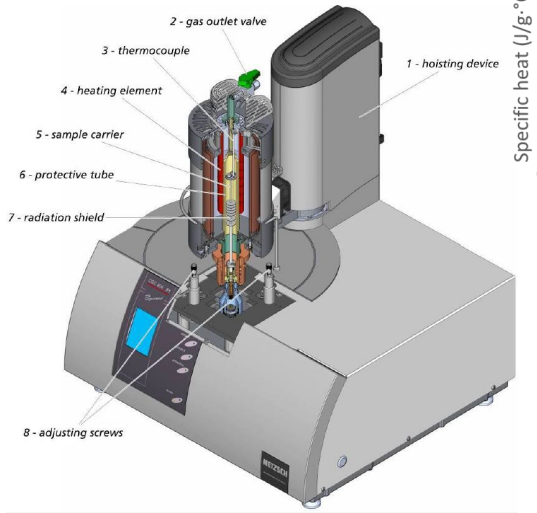


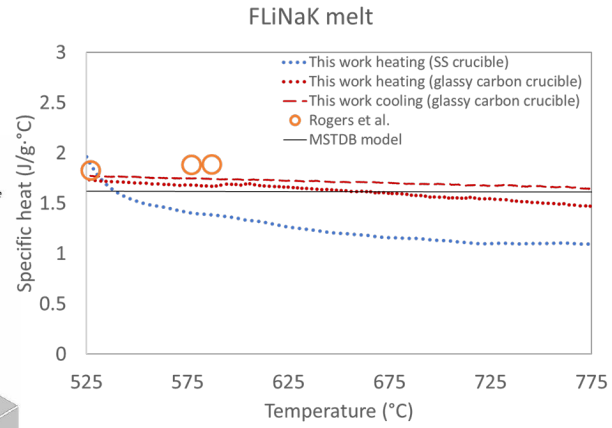




Equivalent to falling-ball optical measurements

Specific Heat





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Pure salts of interest in MSR campaign

The pure salts of interest with their melting temperatures for thermophysical properties

Salt	Melting T (°C)	Salt	Melting T (°C)
$CeCl_3$	822	CeF_3	1432
CsCl	645	CrF_3	1404
LiCl	610	CsF	703
$MgCl_2$	714	KF	858
$NdCl_3$	758	LiF	848
$PuCl_3$	767	NaF	995
$SrCl_2$	873	NdF_3	1377
$ThCl_4$	770	PuF_3	1426
UCl_3	841	SrF_2	1473
UCl_4	590	ThF_4	1110
$ZrCl_4$	437	UF_3	1495
CsI	634	ZrF_4	910
		BeF_2	548

Orange: Immediate goal

Yellow: Near term goal

White: Long term goal

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.

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Binary salt characterizations

- Binary molten salt systems help with modeling of higher order systems
- Molten salts of from tables are impactful for reactor developers
- Experimental or molecular dynamics studies needed

Key
A: Density
B: Viscosity
C: Thermal conductivity
D: Heat capacity

Chloride

KF	B						
LiF	A, B, D	A, B, C, D					
NaF	A, B	A, B, C	A, B, C, D				
ThF4		A, B	A, B, D	A, B			
UF3							
UF4		A, B	A, B	A, B			
ZrF4			A	A, B, D			
	BeF2	**KF**	**LiF**	**NaF**	**ThF4**	**UF3**	**UF4**

Fluoride

KCl	A, B								
LiCl	A	A, B, D							
MgCl2		A, B, D	A, B						
NaCl	A, B	A, B, D	A, D	A, B					
PuCl3									
ThCl4		A			A				
UCl3		A, B	A		A, B				
UCl4		A, B	A	A	A, B				
ZrCl4		A							
	AlCl3	**KCl**	**LiCl**	**MgCl2**	**NaCl**	**PuCl3**	**ThCl4**	**UCl3**	**UCl4**

McMurray, J. et al., 2021. ORNL/SPR-2020/1865.

Thermophysical Modeling

- Provides multicomponent data for reactor modeling

Redlich-Kister expansion density, viscosity and thermal conductivity:

$$\rho_{mix} = \frac{x_A MW_A + x_B MW_B}{\frac{x_A MW_A}{\rho_A} + \frac{x_B MW_B}{\rho_B}} + x_A x_B \left(L_1 + (x_A - x_B) L_2 + (x_A - x_B)^2 \, L_3 + \cdots \right)$$

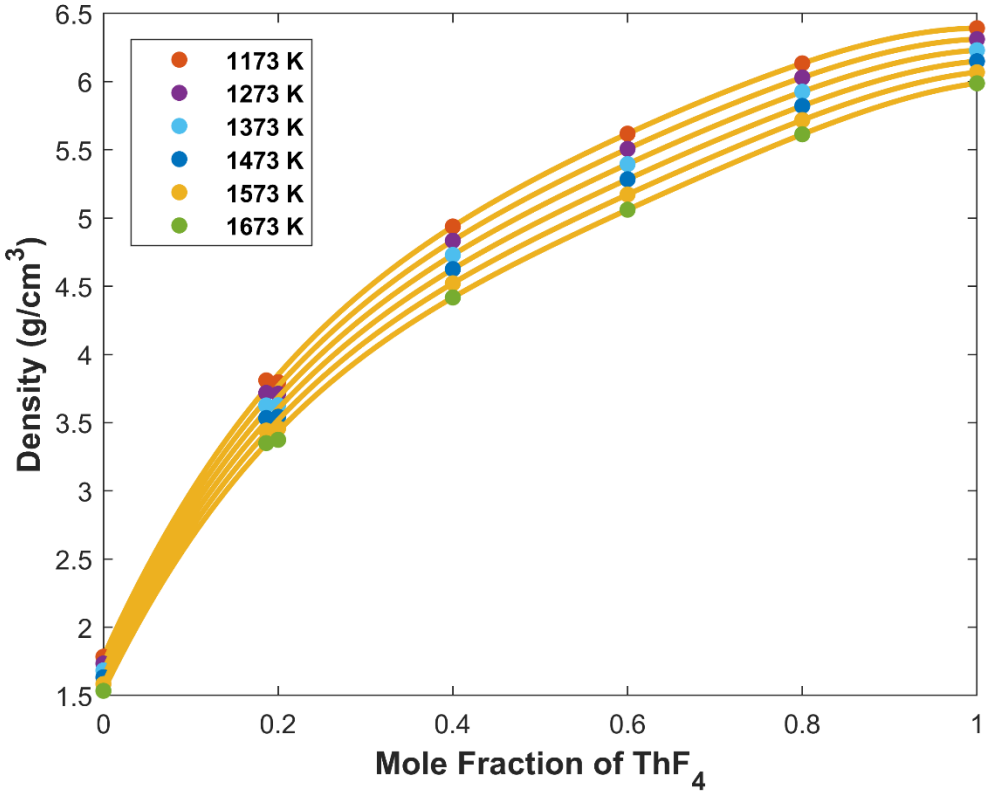
$$\log \mu_{mix} = x_A \log \mu_A + x_B \log \mu_B + x_A x_B \left(L_1 + (x_A - x_B) L_2 + (x_A - x_B)^2 \, L_3 + \cdots \right)$$

$$\lambda_{mix} = x_A \lambda_A + x_B \lambda_B + x_A x_B (L_1 + (x_A - x_B) L_2 + \cdots)$$

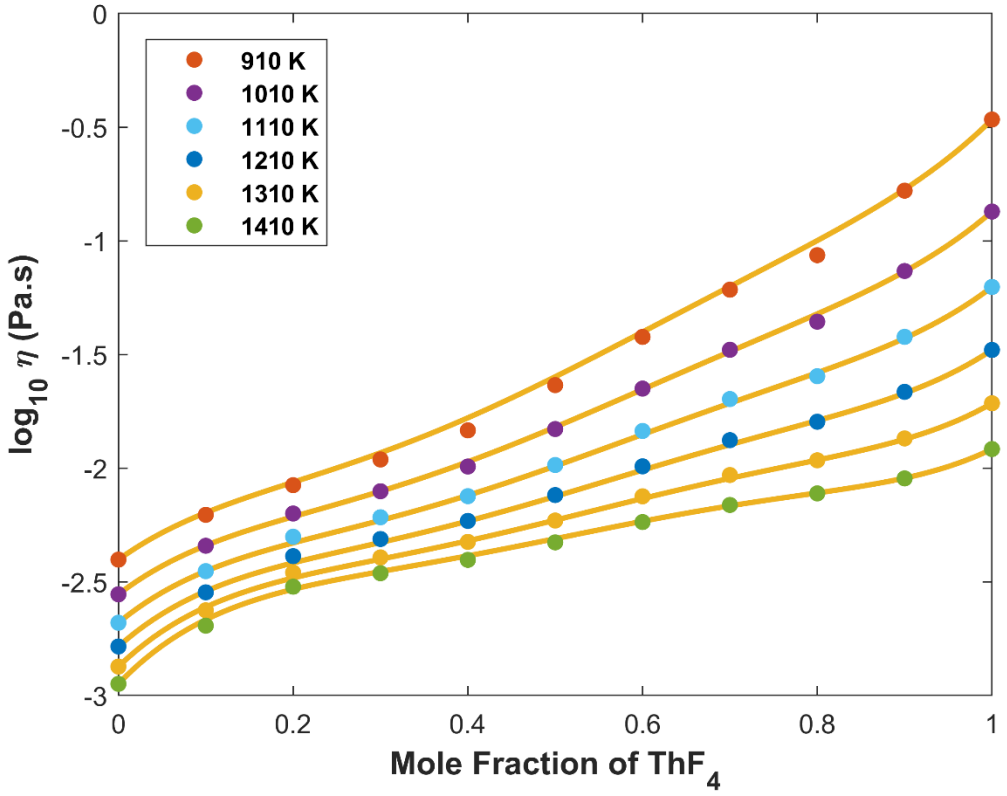
$$L_i = A_i + B_i T$$

Redlich, O.; Kister, A. T.. *Ind. Eng. Chem.* **1948**, *40* (2), 345–348.

LiF-ThF_4 Molten Salt Results



LiF-ThF_4 molten salt system <u>density</u> model

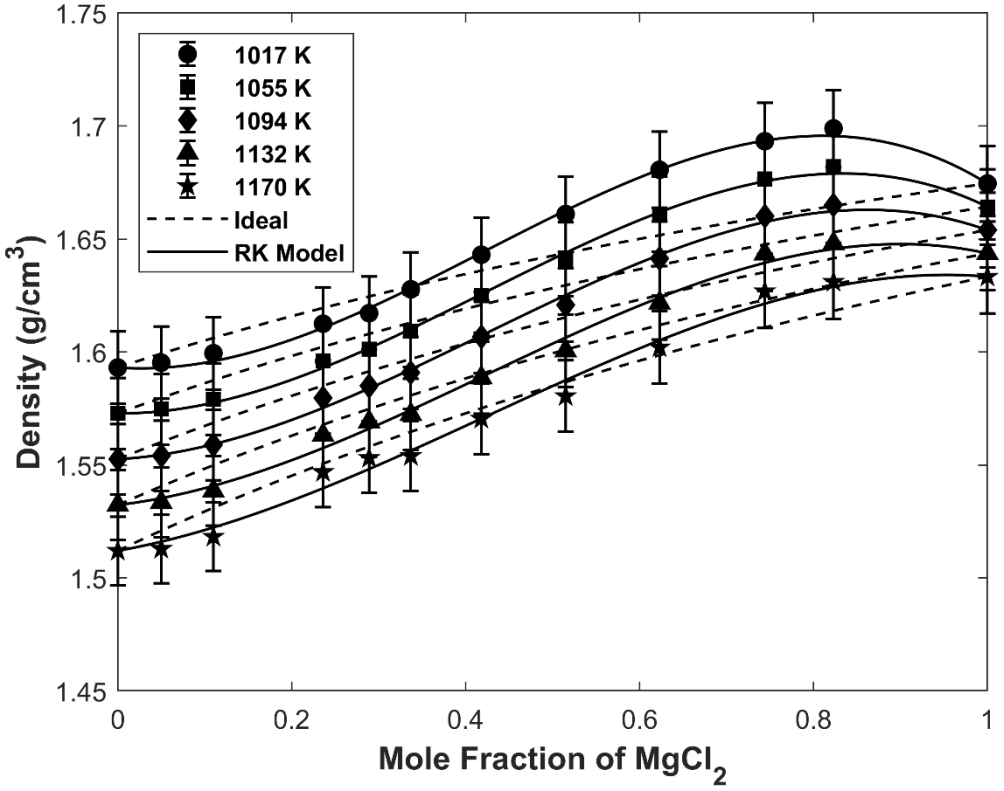


LiF-ThF_4 molten salt system <u>viscosity</u> model

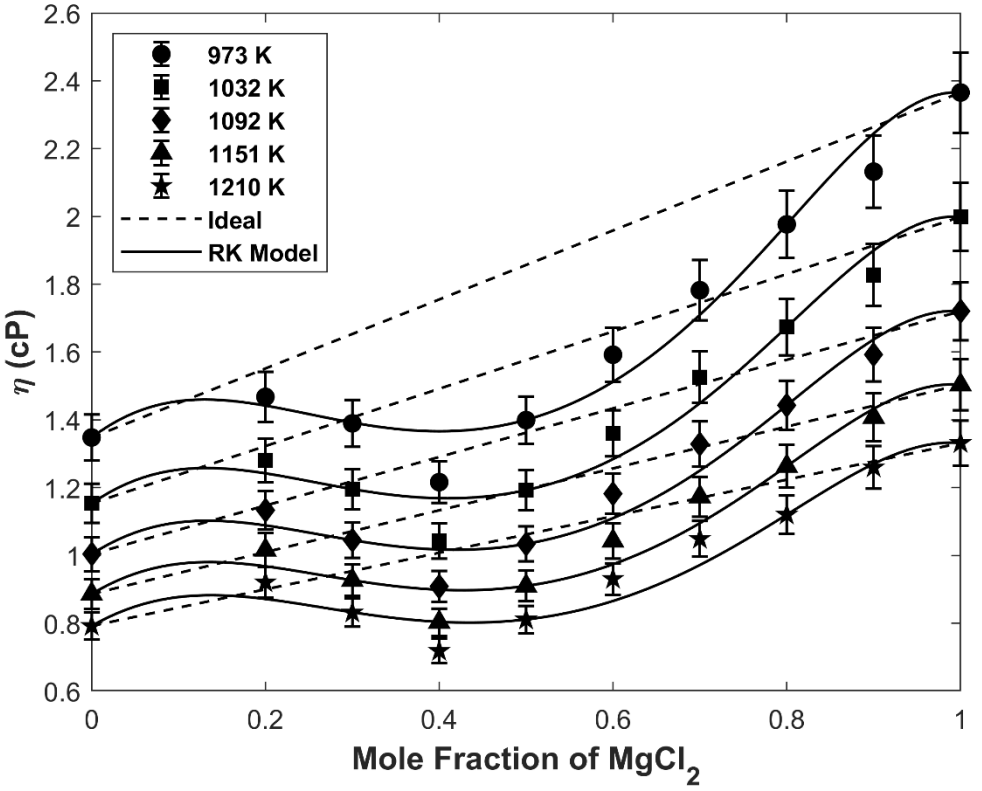
Hill, D. G. et al. *J. Inorg. Nucl. Chem.* **1967**, *29* (1), 241–243.

Chervinskii, Y. F. et al. I. *Zhurnal Fiz. Khimii* **1982**, *56* (8), 1946–1949.

$MgCl_2$-NaCl Molten Salt Results



$MgCl_2$-NACl molten salt system <u>density</u> model



$MgCl_2$-NACl molten salt system <u>viscosity</u> model

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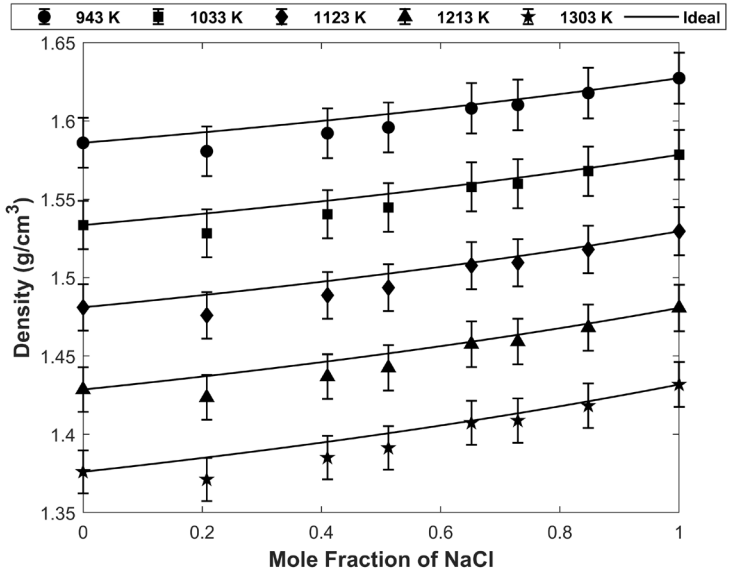
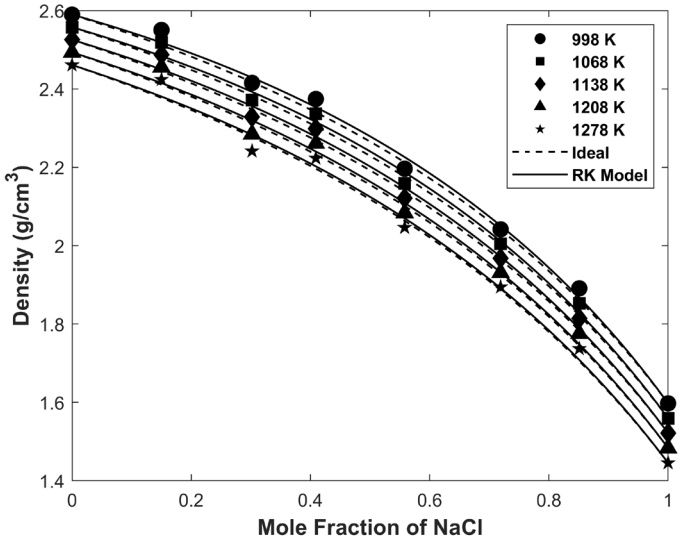
Bondarenko, N. V., and Strelets, Kh. L., J. Appl. Chem. (USSR), 38, 1254 (1965).
Lillebuen, B., Ph.D. Thesis, The Technical University of Norway, Trondheim, Norway, (1969).

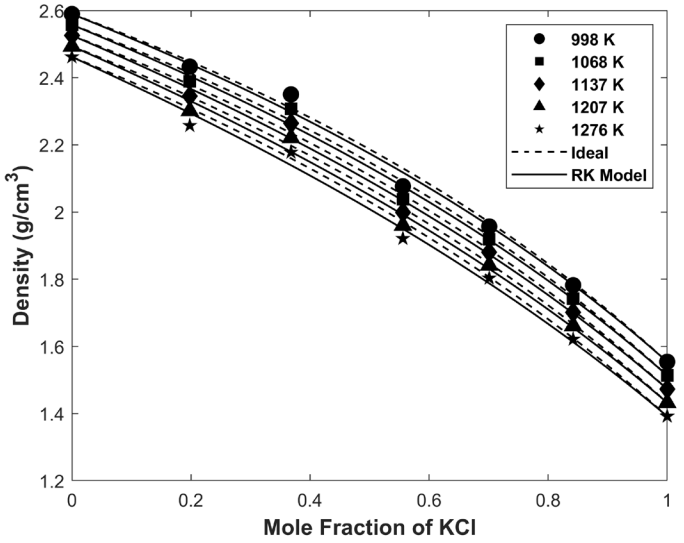
Density of NaCl-KCl-YCl_3 Molten Salts Results



NaCl-KCl molten density: ideal behavior within 1%



NaCl-YCl_3 molten density: RK 1st order



KCl-YCl_3 molten density: RK 1st order

- YCl_3well-known rare-earth fission products in MSRs
- All three binary liquid mixtures behave close-to-ideal in density

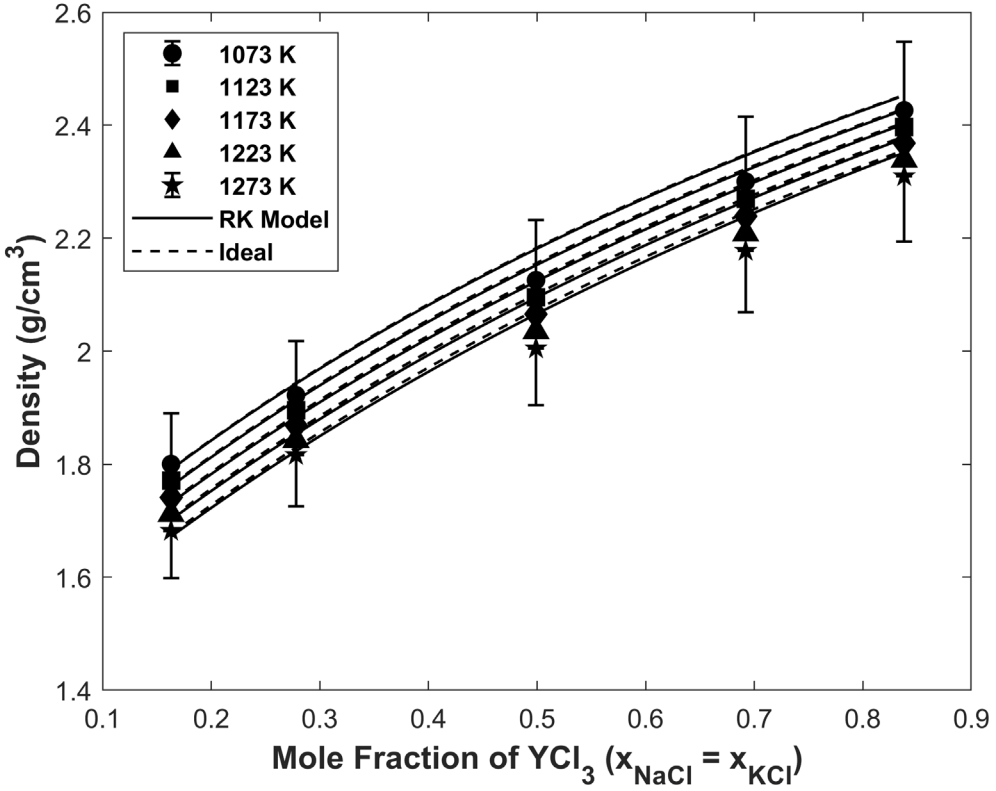
Agca, C.; McMurray, J. W. *Chem. Eng. Sci.* **2022**, *247*, 117086.

Mochinaga, J., Irisawa, K., 1974. Bull. Chem. Soc. Jpn. 47, 364–367.

Van Artsdalen, E.R., Yaffe, I.S., 1955. J. Phys. Chem. 59, 118–127.

Density of NaCl-KCl-YCl_3 Molten Salts Results

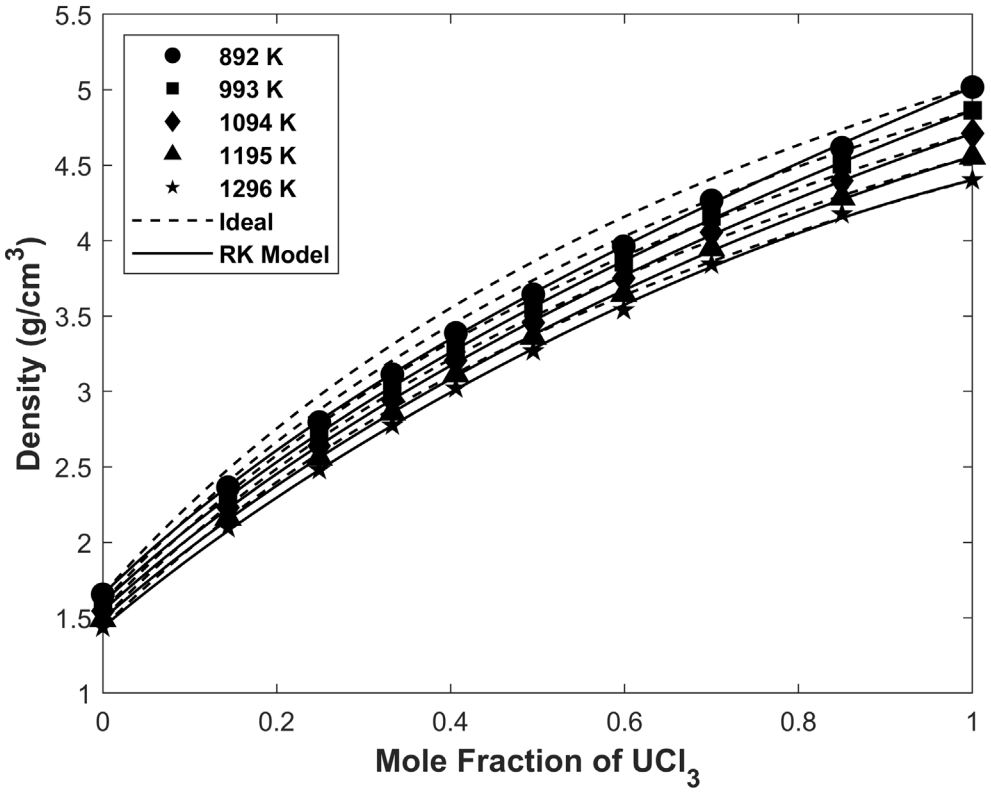
- Muggianu interpolation from binary molten salt interaction parameters
- Good agreement within 2-3%
- Ideal-like behavior for engineering design purposes



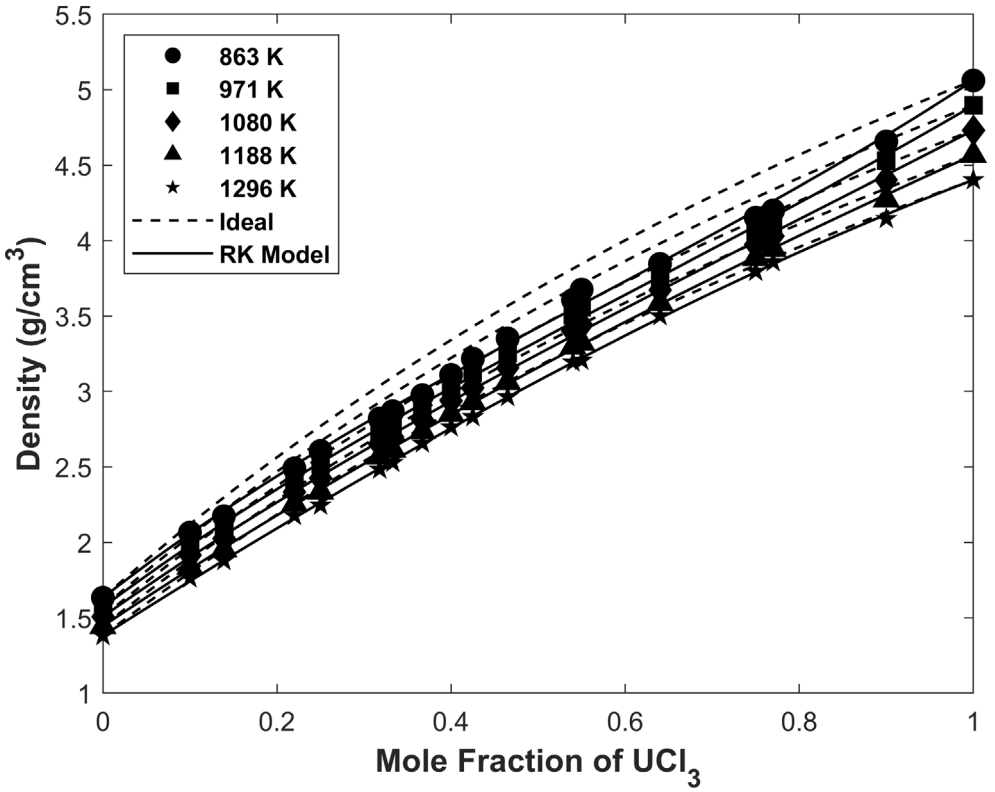
$$\rho_{ex} = x_A x_B \sum_{j=1}^{n} L_j (x_A - x_B)^{j-1} + x_A x_C \sum_{j=1}^{n} L_j (x_A - x_C)^{j-1} + x_B x_C \sum_{j=1}^{n} L_j (x_B - x_C)^{j-1}$$

Agca, C.; McMurray, J. W. *Chem. Eng. Sci.* **2022**, *247*, 117086.
Muggianu, Y.-M. et al., 1975. J. Chim. Phys. 72, 83–88.
Mochinaga, J., Irisawa, K., 1974. Bull. Chem. Soc. Jpn. 47, 364–367.

Density of NaCl-KCl-UCl_3 Molten Salt Results



NaCl-UCl_3 molten salt density: RK 2nd order



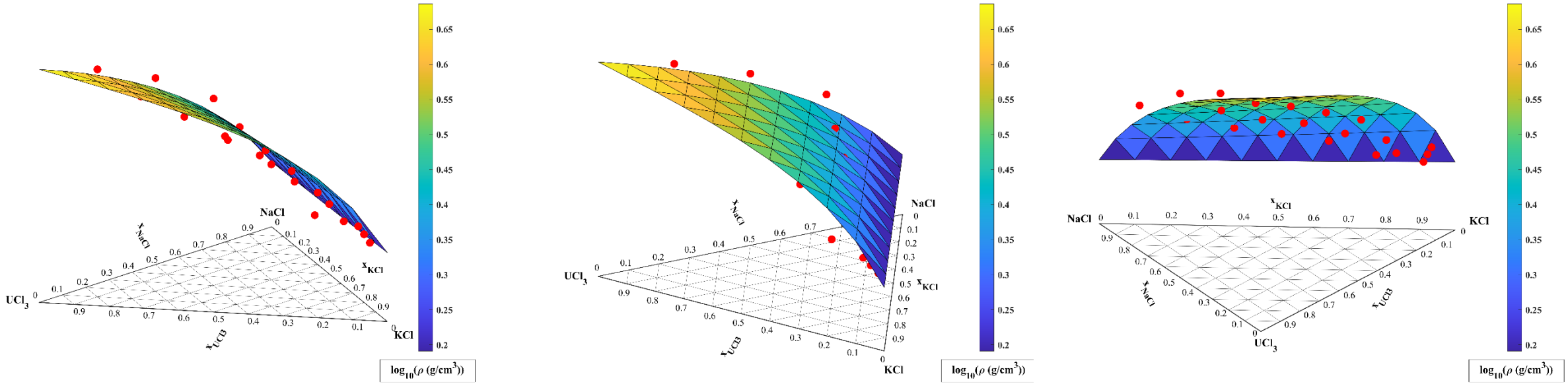
KCl-UCl_3 molten salt density: RK 2nd order

Agca, C.; McMurray, J. W. *Chem. Eng. Sci.* **2022**, *247*, 117086.

Desyatnik, V. N. et al. Sov. At. Energy 1975, 39 (1), 649–651.

Desyatnik, V. N. et al. Zhurnal Fiz. khimii 1976, 50 (10), 2522–2525.

3D visualization of the Density of NaCl-KCl-UCl_3



- NaCl-KCl-UCl_3 system at 1000 K shows a good agreement with Katyshev et al. (1983)

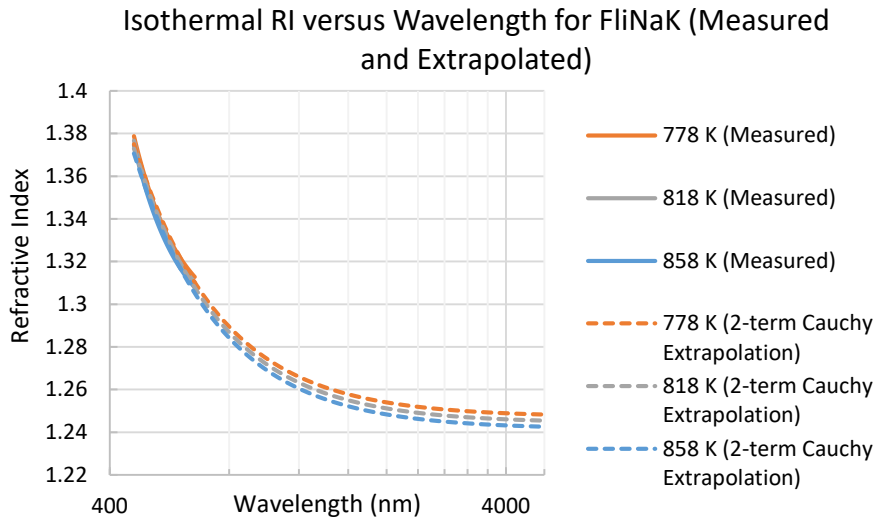
OAK RIDGE National Laboratory

Agca, C.; McMurray, J. W. *Chem. Eng. Sci.* **2022**, *247*, 117086.
Katyshev, S.F. et al. 1983. J. Appl. Chem. USSR 56, 2000–2002.

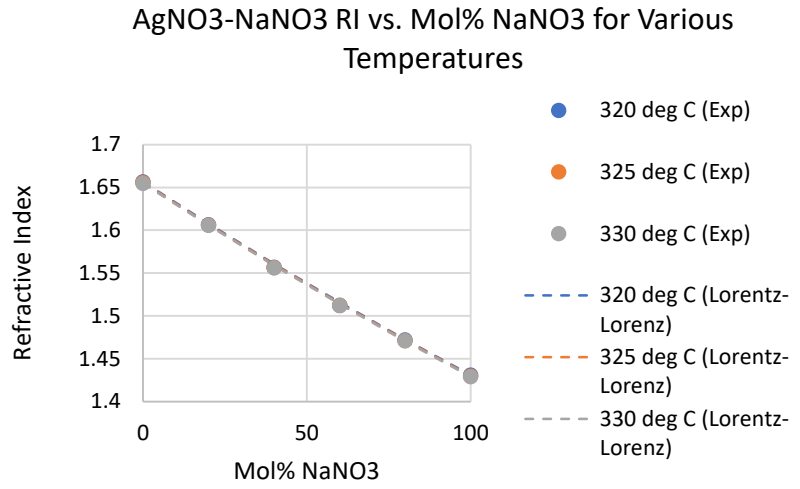
Optical Property Library Development

- To make accurate thermal conductivity measurements of molten salts, knowledge of the salts optical properties must be known or approximated
- A library of molten salt optical properties is being developed to provide a user with a measured or approximated value of refractive index (RI) or absorption coefficient
  - So far, a significant amount of RI data has been added to the library
- Methods of approximating RI values relevant to radiant heating are being investigated
  - Most measured values of RI have been taken in the visible range
  - These RI values are wavelength dependent, so obtaining accurate RI values for the blackbody spectrum requires adjustments to measured data
  - Cauchy's transmission equation has been utilized for these corrections
- Approximating the RI of a salt mixture can be achieved by use of the Lorentz-Lorenz equation assuming the pure salt RIs are known

Application of Cauchy's Equation

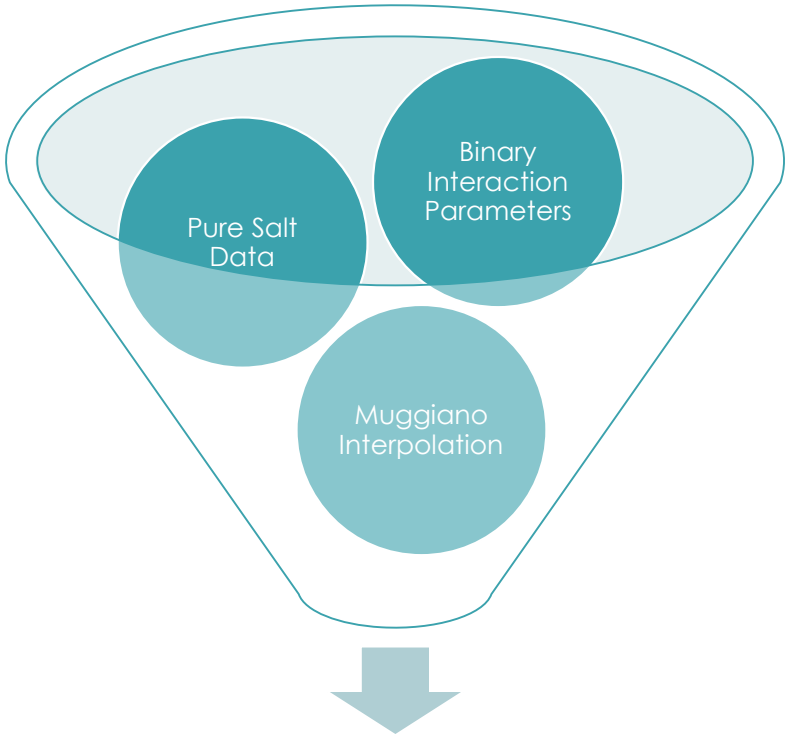


Application of Lorentz-Lorenz equation



Molten Salt Density Calculations

- The work is being transferred and consolidated from MATLAB into Python
  - Closed-source to open-source
  - Several scripts to one script
  - Enables higher user-friendliness
- The python code has been validated for several salt mixtures; it provides identical outputs as the MATLAB scripts
- More ternary salts are being identified to validate the use case of the estimation method
  - These salts are of interest to industry
  - Currently investigating NaF-LiF-ZrF4 as the necessary data has been identified
  - Data on these ternary salts for method validation is limited



One user-friendly script

Molten Salt Thermophysical Properties API

Shane Henderson, Robert Lefebvre

- Under active development
- Provides a stable C++ interface for obtaining supported properties (density, viscosity, heat capacity, and thermal conductivity)
  - Can be extended to provide access to alternate and/or additional data models without affecting client codes.
- Seeks to provide results which mirror experiment while being robust in the absence of data.
  - Falls back on ideal mixing
- Support for standalone use provided via python bindings
  - Could be extended to additional bindings

Henderson, S. et al. *Saline: An API for Thermophysical Properties, ORNL/TM-2021/2239*; 2021.

Conclusions and Future Work

- A framework has been developed and path forward proposed for multicomponent salt thermal property modeling
- Fundamental pure component and binary mixture data are used as inputs to populate the MSTDB
- Key data gaps have been identified and systems for computational and experimental studies have been selected
- An API has been developed for coupling the MSTDB-TP to NEAMS and other codes for multiphysics modeling and simulation


Questions?
Dianne Ezell
bullnd@ornl.gov