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

Clean. Reliable. Nuclear.

Overview of Databases

MSR Campaign Review Meeting

26 & 27 April 2022

T. Besmann, Univ. of South Carolina

N. Dianne Bull Ezell, ORNL

NEAMS NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

Molten Salt Reactor PROGRAM

MSTDB-TP Development

- Email: mstdb@ornl.gov
- URL: code.ornl.gov/neams/mstdb-tp

OAK RIDGE National Laboratory

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.

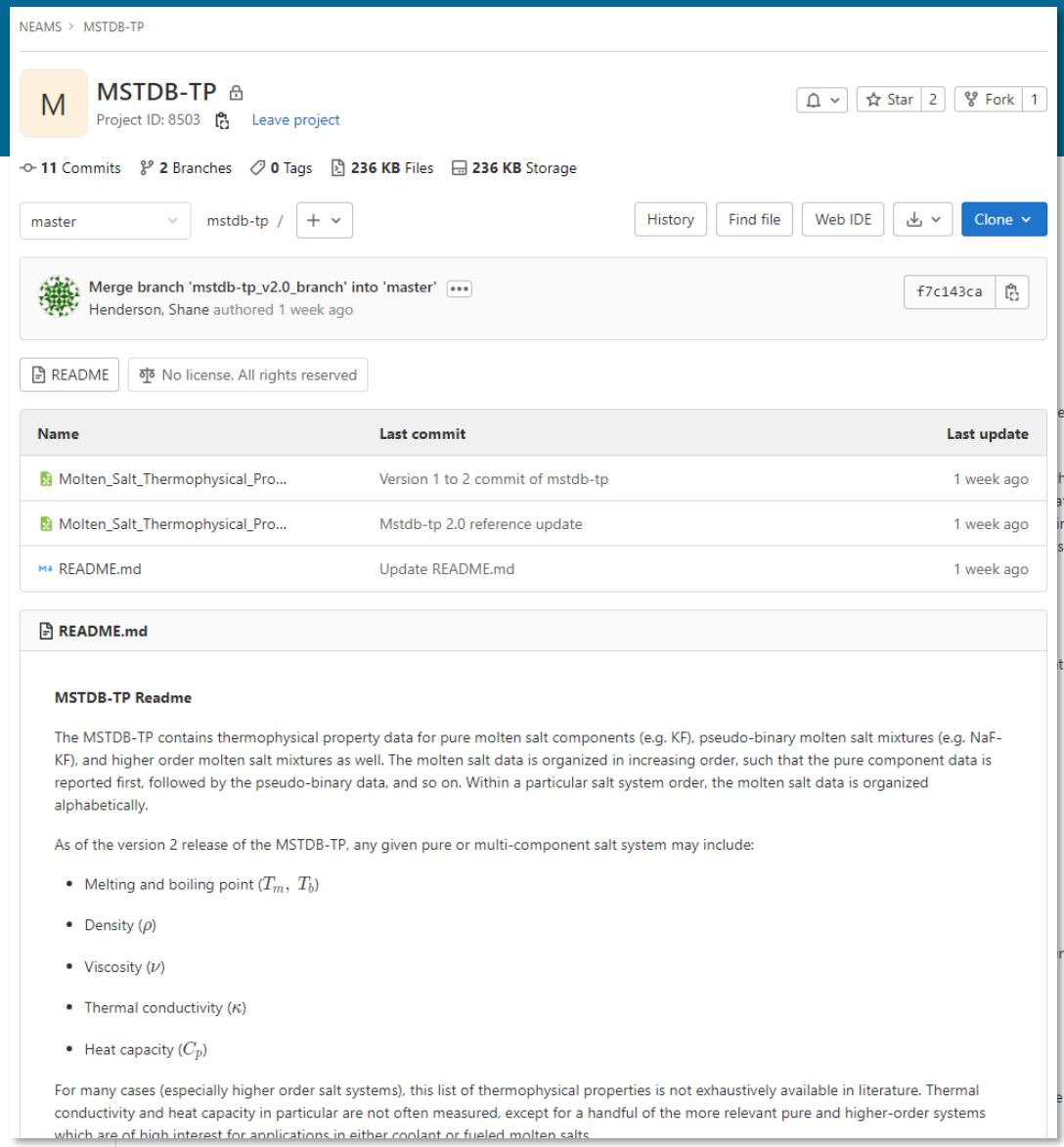
MSTDB-TC thermodynamic information resides in files in the "Chemsage" .dat (ASC II) format for use with the FactSage® commercial package of thermodynamic codes and compatible with the open-source equilibrium code Thermochimica.

- 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



NEAMS > MSTDB-TP

M **MSTDB-TP**

Project ID: 8503 Leave project

Star 2 Fork 1

11 Commits 2 Branches 0 Tags 236 KB Files 236 KB Storage

master mstdb-tp / + History Find file Web IDE Clone

Merge branch 'mstdb-tp_v2.0_branch' into 'master'

Henderson, Shane authored 1 week ago f7c143ca

README No license. All rights reserved

Name	Last commit	Last update
Molten_Salt_Thermophysical_Pro...	Version 1 to 2 commit of mstdb-tp	1 week ago
Molten_Salt_Thermophysical_Pro...	Mstdb-tp 2.0 reference update	1 week ago
README.md	Update README.md	1 week ago

README.md

MSTDB-TP Readme

The MSTDB-TP contains thermophysical property data for pure molten salt components (e.g. KF), pseudo-binary molten salt mixtures (e.g. NaF-KF), and higher order molten salt mixtures as well. The molten salt data is organized in increasing order, such that the pure component data is reported first, followed by the pseudo-binary data, and so on. Within a particular salt system order, the molten salt data is organized alphabetically.

As of the version 2 release of the MSTDB-TP, any given pure or multi-component salt system may include:

- Melting and boiling point (T_m, T_b)
- Density (ρ)
- Viscosity (ν)
- Thermal conductivity (κ)
- Heat capacity (C_p)

For many cases (especially higher order salt systems), this list of thermophysical properties is not exhaustively available in literature. Thermal conductivity and heat capacity in particular are not often measured, except for a handful of the more relevant pure and higher-order systems which are of high interest for applications in either coolant or fueled molten salts.

For the thermophysical properties in the database, associated applicable temperature ranges, uncertainties, and references to the base literature are provided. In some cases, where uncertainties are difficult to quantify based on limited detail in the reference literature, a "*" sign follows the uncertainty, indicating that this listed uncertainty is representative of a generally accepted upper bound for that particular thermophysical property measurement.

MSTDB-TC Development

Update to CLAK V2
Ard, Johnathon authored 1 month ago

714f5047

Name	Last commit	Last update
.gitlab/issue_templates	Adding new-data-package checklist issue template.	1 year ago
models	Update to CLAK V2	1 month ago
README.md	Update README.md for MSAX-CLAK	1 month ago

README.md

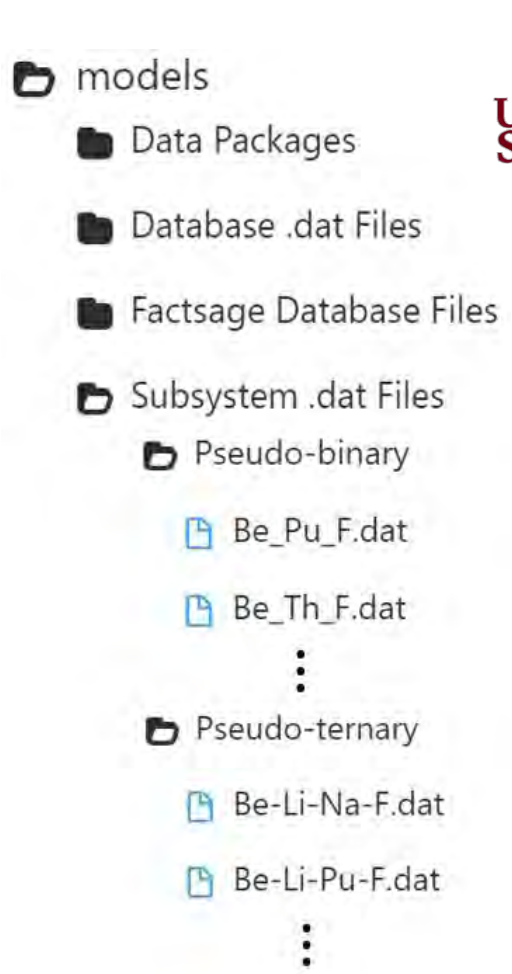
MSTDB

The molten salt thermochemical database (MSTDB).

MSTDB will be a publicly available database of thermodynamic models and values for fluoride and chloride molten salt components and related systems of interest with respect to molten salt reactor technology. These include fuel or coolant salts, consequential fission product and transuranic elements, contaminants such as air and moisture, and likely corrosion product elements such as nickel and chromium. Phases will include gas/vapor, liquids (e.g., molten salts, noble metals), and solid compounds. The database will consist of one or more files constituting the entire developed database in the "Chemsage" format accessible with the FactSage® commercial package and compatible with the open source equilibrium code Thermochimica (i.e., in the .dat format).

The models and values provided within MSTDB will be obtained through combinations of literature-reported information, first principles calculations, and experimental measurements. These will be used to a greater or lesser extent as needed in assessments for binary, ternary, and higher order systems. A system is said to be assessed when sufficient experimental and theoretical data are available to optimize adjustable thermochemical values and parameters for each model and species so as to represent each phase in that system. In essence, a system is assessed when models and values appropriately reproduce the phase equilibria (phase diagram) and attendant values such as heat capacity and vapor pressures.

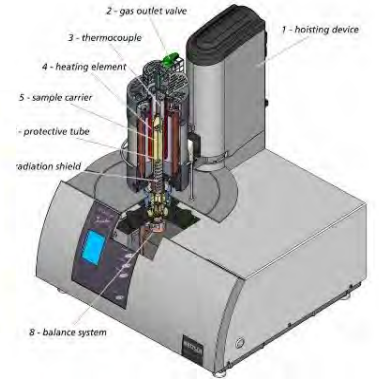
Granted access covers both databases (on same GitLab)

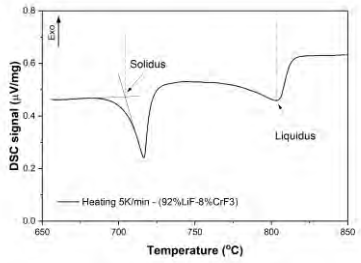


MSTDB-TC Methodologies: Assessments Generate Accurate Thermodynamic Values/Parameters

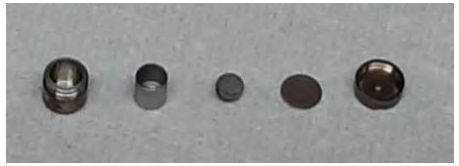
- Data mining
- First principles calculations
  - Determining energy of formation for crystalline phases
  - Coordination numbers to improve molten salt models
- Experimental determination of key values
  - DSC for phase transitions (solidus, liquidus…)
  - XRD for phase identification
- CALPHAD assessments: Uses all appropriate system properties to fit to phase thermodynamic models
  - Yields generally applicable model values/parameters
  - Reproduce phase equilibria and thermal properties

DSC and XRD measurements

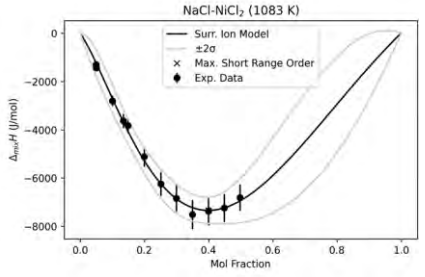


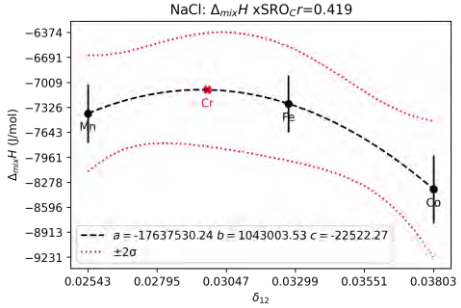


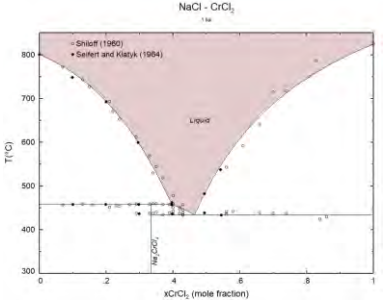
Netzsch SS sealable DSC crucible w Ni liner



Correlations based on heat of mixing

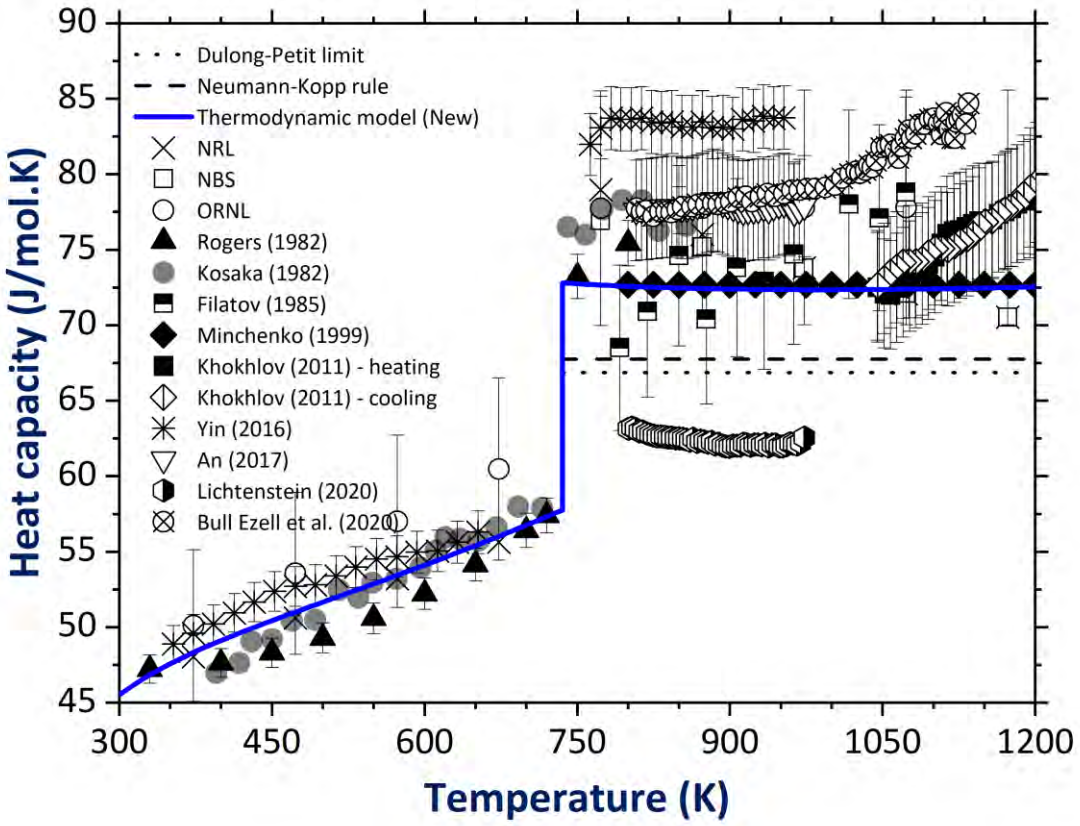






Issues in Base System Values Are Challenging

FLiNaK liquid Cp value results vary and needed to be reconciled



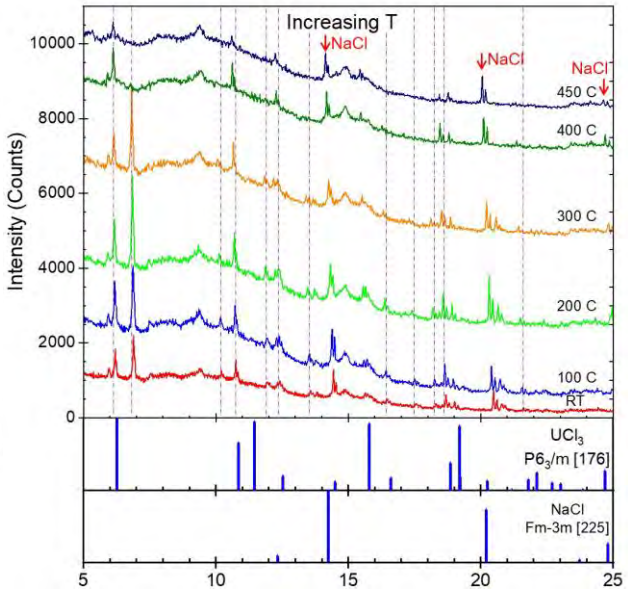
Incongruent melting compound NaU_2Cl_7 or $Na_3U_5Cl_{18}$ may exist

Ionic potential (IP) correlations

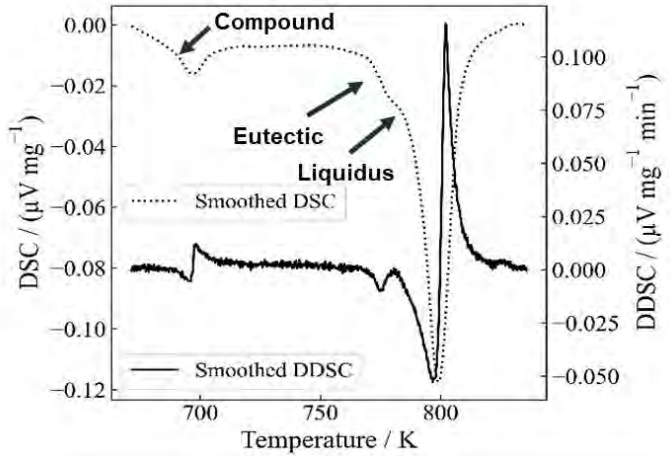
System	IP_{M+}/IP_{Ln3+}	System type
$LiCl\text{-}LaCl_3$	0.478	Eutectic
$LiCl\text{-}NdCl_3$	0.448	Eutectic
$LiCl\text{-}TbCl_3$	0.416	$LiTb_2Cl_7$
$LiCl\text{-}HoCl_3$	0.402	Li_3HoCl_6[a]
$NaCl\text{-}NdCl_3$	0.325	$Na_3Nd_5Cl_{18}$[a,b]

More Compounds

[a] Incongruently melting
[b] Incorrectly reported as Na_3NdCl_6



DSC indicates endothermic peak near 688K: Intermediate compound



DSC at 33.4mol% UCl_3 (5 K min^{-1})

HT XRD reveals high temperature intermediate phase

Linked Data Packages Provided 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	

Tested 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\

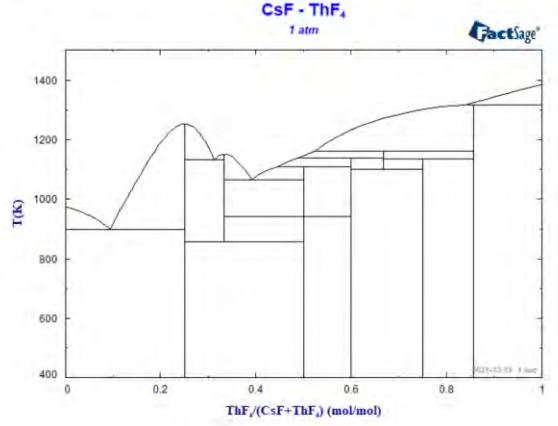
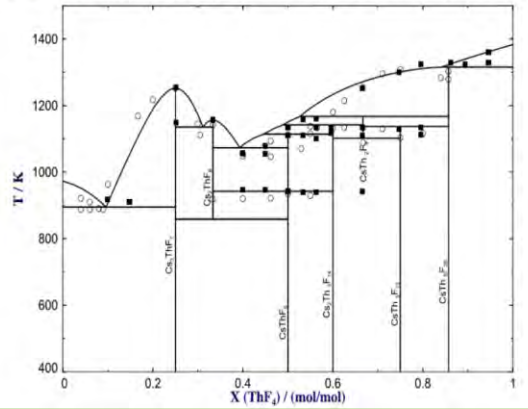


Fig. 31b - Published figure from Ref[9] saved in C:\FactSage80\MSTDB\PD_Macro\Lit
Please see Excel data package for this system for additional information.



103: LiF-NaF-PuF3

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

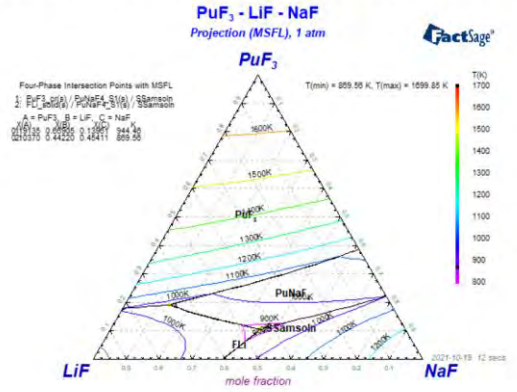
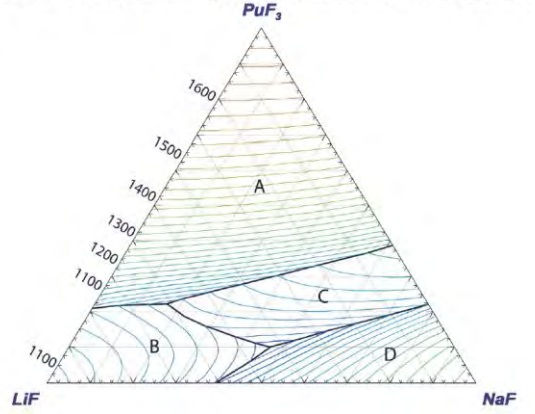


Fig. 103b - Published figure from Ref[3] saved in C:\FactSage80\MSTDB\PD_Macro\Lit
Please see Excel data package for this system for additional information.

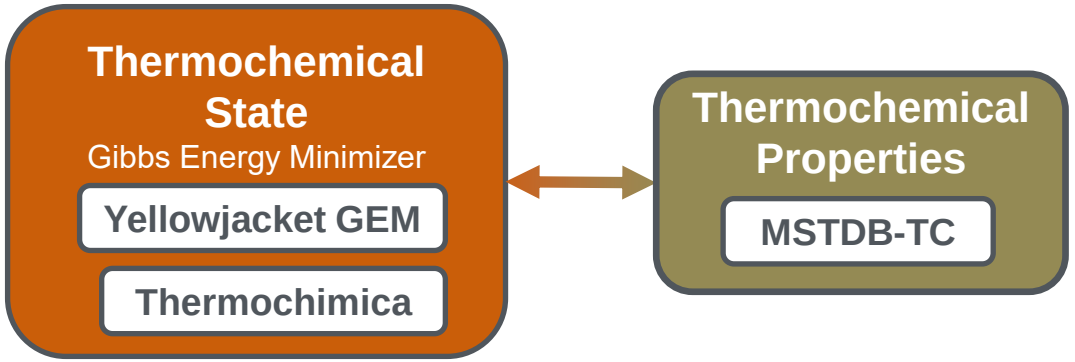


MSTDB-TC Ver. 1.2 content

- **Fluoride-based Systems**
  - Be-Ca-Ce-Cs-K-La-Li-Mg-Na-Ni-Nd-Pu-Rb-Th-U-F
  - 108 stoichiometric compounds
  - 45 pseudo-binary subsystems
  - 26 pseudo-ternary subsystems
  - Higher order systems
    - LiF-NaF-RbF-LaF_3
    - LiF-NaF-CaF_2-LaF_3
    - LiF-NaF-BeF_2-ThF_4-UF_4-PuF_3
    - NaCl-$MgCl_2$-UCl_3-$PuCl_3$
  - 22 solid solutions

- **Chloride-based Systems**
  - Cs-K-Li-Mg-Na-Pu-U-Cl
  - 37 stoichiometric compounds
  - 13 pseudo-binary subsystems
  - 1 pseudo-ternary subsystem
  - Higher order system
    - NaCl-$MgCl_2$-UCl_3-$PuCl_3$
  - 3 solid solutions
  - Models for excess K and Mg in solution

MSTDB-TC provides Gibbs functions for calculations in simulation codes



New Content in Ver. 2: Expected June 2022

Highlighting corrosion and cesium- and iodine- containing systems

Additional Systems

- NaF-NaCl
- KF-KCl
- CsF-CsCl
- KCl-KI
- CsF-CsI
- CsCl-CsI
- NaCl-NaI
- KCl-KI
- BeF_2-BeI_2
- KF-KI
- CsF-BeF_2
- $CrCl_2$-$MgCl_2$
- $CrCl_3$-(Na, K, Mg)Clx
- KCl-$MgCl_2$-NaCl
- $FeCl_2$-KCl-NaCl
- FeCl2-$MgCl_2$-NaCl
- KCl-NaCl-$NiCl_2$
- KCl-$MgCl_2$-$NiCl_2$

Reassessed Existing Content

- LiF-CsF
- NaF-CsF
- KF-CsF
- CaF_2-LaF_3
- CaF_2-ThF_4
- NaF-CeF_3
- LiF-CaF_2-ThF_4

MSTDB-TP Database Entries

- **MSTDB-TP Version 2.0 in-progress (available April 2022)**
- Type of data (along with references and uncertainty)
  - Melting temperature
  - Boiling temperature
  - Density
  - Optical Properties
  - Viscosity
  - Thermal Conductivity
  - Heat capacity
- 273 entries currently: 33 pure, 214 binaries, 20 ternaries & 6 quaternaries

Component Data

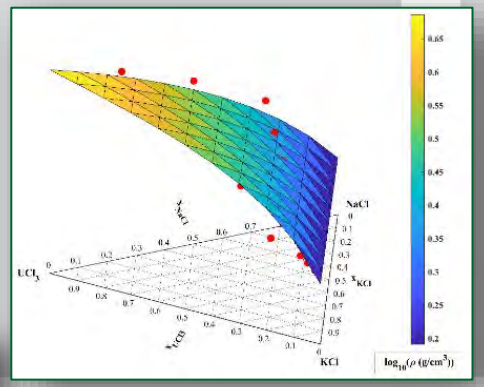
- Estimation from databases
  - Multicomponent system behavior estimated by extrapolation of lower order systems (pseudo-binary)
  - Databases contain pure and binary mixture properties

Modeling

- Redlich-Kister Expansion
  - Corrects for interaction in binary system
  - Accuracy depends on pure and binary component data

Extrapolation

- Extrapolate expansion and fit to higher order systems
  - Ternaries
  - Quaternaries



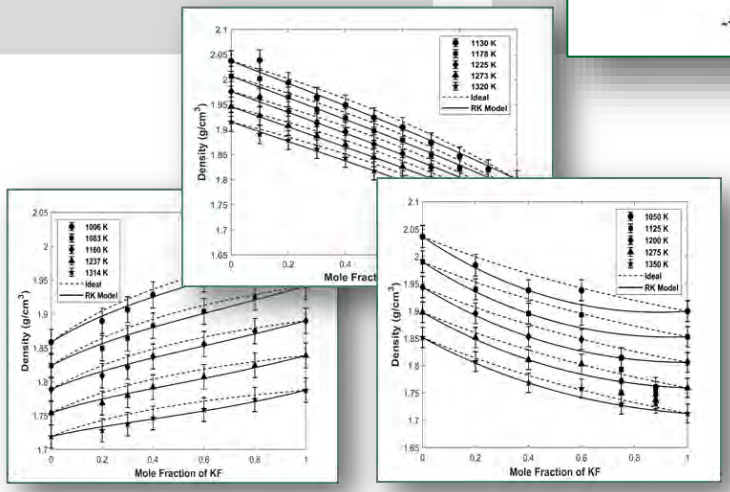
MSTDB-TP

- Database of models/ model parameters that will represent salt solution thermal property behavior as a function of temperature and composition

Saline

- Application Programming Interface
- Provides a stable C++ interface for obtaining supported properties

Pure Salt	Density Equation (g/cm^3), T in K
KF	2.6616 – 6.6500 x 10^{-4} T
LiF	2.3289 – 4.6803 x 10^{-4} T
NaF	2.6820 – 6.1510 x 10^{-4} T



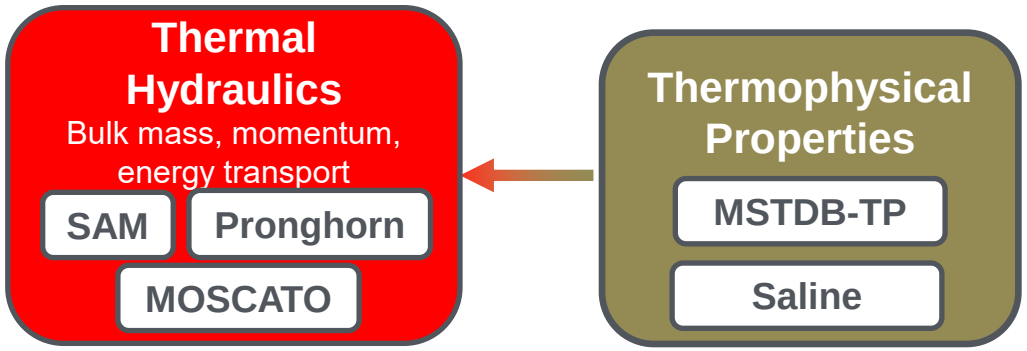
- Melting/Boiling Temperatures
- Density
- Thermal conductivity
- Viscosity
- Heat Capacity
- Optical Properties

MSTDB-TP

```
#include "default_data_store.hh"
#include "thermophysical_properties.hh"

// Construct the default data store object
Default_Data_Store d;

// Load the default data
d.load();

// Construct the thermophysical properties object
Thermophysical_Properties tp;

// Initialize it with the data store
tp.initialize(&d);

// Pick a composition
tp.setComposition({"LiF","NaF","KF"},{0.465,0.115,0.42});

// Obtain data using temperature in Kelvin
double density = tp.rho(900);
double viscosity= tp.mu(900);
double thermal_conductivity = tp.k(900);
double heat_capacity = tp.cp(900);
```

Molten Salt Thermophysical Properties API - Saline

- 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-2021/2238*

Questions/Discussion