Agenda

Training/Workshop for the
Molten Salt Thermal Properties Databases

Molten Salt Thermal Properties Working Group
University of South Carolina
Virtual, April 25, 2023

All times are EDT

10:00 am	**Introductions**	Dianne Ezell, ORNL Ted Besmann, USC
10:05 am	**DOE programs supporting databases development**	Chris Stanek, NEAMS Natl. Tech. Director
	Creation and application of MSTDB-Thermochemical	Ted Besmann, USC
10:25 am	MSTDB-TC development	Juliano Schorne-Pinto, USC
10:45 am	MSTDB-TC quality assessment	Max Poschmann, Ontario Tech/CNL
11:05 am	Using MSTDB-TC with Factsage and examples	Ted Besmann, USC
11:25 am	Use of MSTDB-TC with Thermochimica and examples	Markus Piro Ontario Tech
11:45 am	Using MSTDB-TC with a MOOSE-based Model of Corrosion of Structural Materials by Molten Salt at the Mesoscale	Mike Tonks, U. Florida
12:10 pm	**Break**	
12:30 pm	MSTDB-TC: Molten salt chemistry applications for development of the Kairos Power FHR.	Jake McMurray, Kairos
	Creation and application of MSTDB-Thermophysical	Dianne Ezell, ORNL
1:00 pm	MSTDB-TP development, expansion, and control processes	Tony Birri, ORNL
1:20 pm	Demonstration of a user interface for MSTDB-TP	Nick Termini, ORNL
1:40 pm	MSTDB-TP applications with Saline and examples	Shane Henderson, ORNL
1:55 pm	Applications of MSTDB-TP in NEAMS for modeling of MSRs	Bob Salko, ORNL
2:15 pm	Sensitivity analysis of thermophysical properties of molten salts using a MSDR model in TRANSFORM	Sarah Creasman, UTK
2:35 pm	**General Discussion & Wrap-up**	
3:00 pm	**Adjourn**	

General Atomics SmartState Center for Transformational Nuclear Technologies

MSTDB-TC DEVELOPMENT

J. Schorne-Pinto, J. C. Ard, J. A. Yingling, M. Aziziha, C. M. Dixon,
J. Paz Soldan Palma, K.E Johnson, A. M. Mofrad, M. S. Christian, T. M Besmann

Nuclear Engineering Program, Mechanical Engineering Department, University of South Carolina

NEUP Nuclear Energy University Program
U.S. Department of Energy
NEAMS NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

UNIVERSITY OF South Carolina

U.S. DEPARTMENT OF ENERGY
Office of NUCLEAR ENERGY

CONTEXT

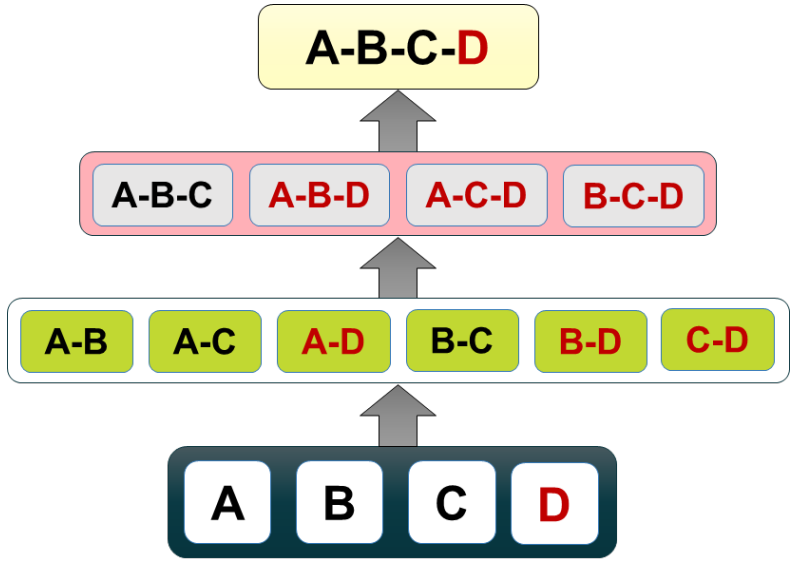
- Reliable **thermal properties** are required for the **entire operating temperature range** and potential overtemperature for MSRs
- These properties are often dependent on both **composition and temperature**
- In particular, the ability to **compute the behavior of the solid, liquid, and vapor phase for multi-component systems** is essential for describing the **chemical behavior** of molten salts in applications

THE CALPHAD METHOD

Principle:

- Computational method for calculating multicomponent phase diagrams
- Phase diagram is a graphical representation of thermodynamic properties
- Thermodynamic equilibrium at temperature (T), pressure (p), number of moles (N) is calculated by minimizing the total Gibbs energy (G) of the system

Requiring **extensive set of Gibbs Energy functions** for **each component** of a system and **its interaction** with other components stored in a database



Need use a code to compute minimum total G of a system

FactSage™ Thermo-Calc Software

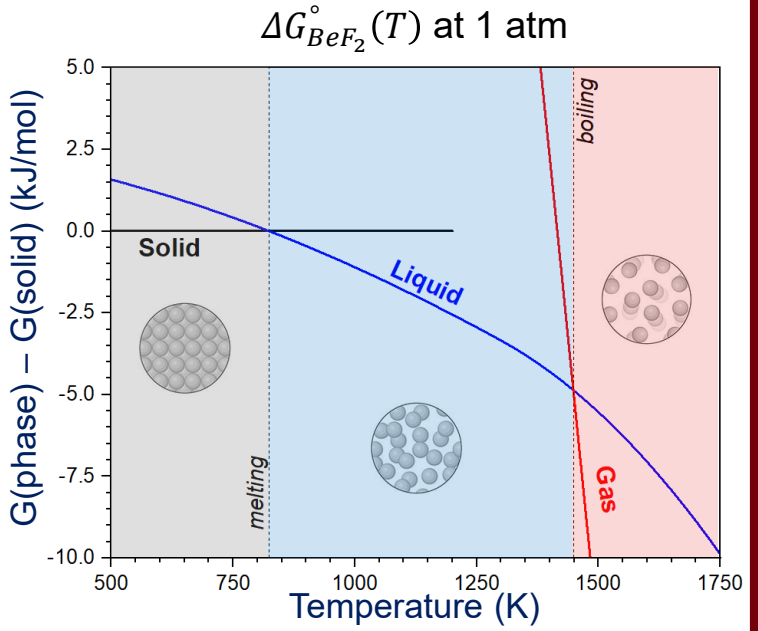
Thermochimica

THE CALPHAD METHOD

Phases with fixed composition (**stoichiometric**):

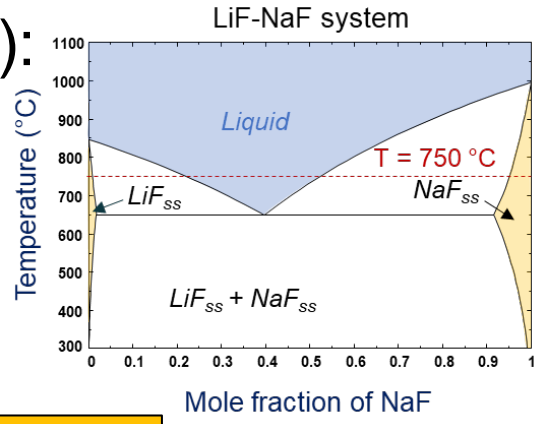
$$\Delta G_i^\circ(T) = \Delta H_{298.15}^\circ(i) + \int_{298.15}^{T} C_{P_i}^\circ(T)\,dT - T\left(S_{298.15}^\circ(i) + \int_{298.15}^{T} \frac{C_{P_i}^\circ(T)}{T}\,dT\right)$$

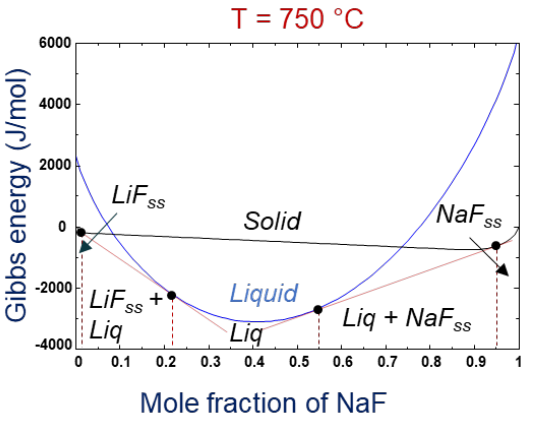
- $\Delta H_{298.15}^\circ(i)$ is the standard enthalpy of formation
- $S_{298.15}^\circ(i)$ is the standard entropy
- $C_{P_i}^\circ(T)$ is the isobaric heat capacity



Phases with variable composition (**solution**):

$$\Delta G_m^\circ(T) = \underbrace{\sum_{i=1}^{n} x_i \Delta G_i^\circ(T)}_{\text{Reference}} + \underbrace{RT\sum_{i=1}^{n} x_i ln(x_i)}_{\text{Ideal}} + \underbrace{\Delta G_m^{xs}(T)}_{\text{Excess}}$$





Adjusted to obtain the best representation of the experimental data

MOLTEN SALT THERMAL PROPERTIES DATABASE - THERMOCHEMICAL

MSTDB-TC consists of a **library of Gibbs energy functions** within relevant **solution** models for salt systems including compounds, **solid solutions, salt melt, and vapor species**

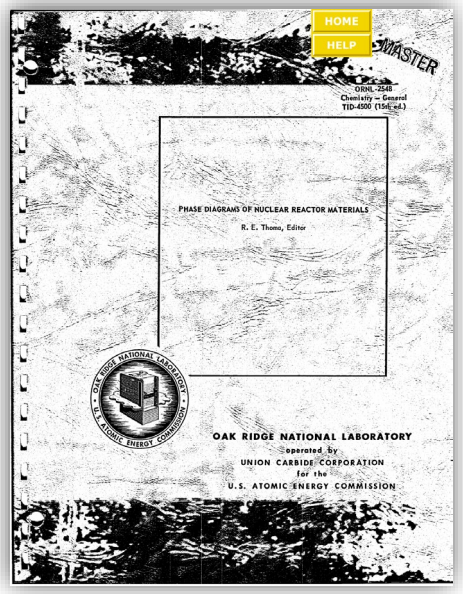
Constant revisited and updated, increasing the number of evaluated systems:

	Fluorides	**Chloride**	**Iodides**
Alkali metals	LiF, NaF, KF, RbF, CsF	LiCl, NaCl, KCl, RbCl, CsCl	LiI, NaI, KI, CsI
Alkaline earth metal	BeF_2, CaF_2, **SrF_2, BaF_2**	$MgCl_2$, $CaCl_2$	BeI_2, MgI_2
Transition metals	NiF_2, CrF_3	$CrCl_2$, $CrCl_3$, $FeCl_2$, $FeCl_3$, $NiCl_2$	-
Other metals	**YF_3, ZrF_4**	$AlCl_3$	-
Lanthanides	LaF_3, CeF_3, NdF_3, **PrF_3**	$CeCl_3$, **$LaCl_3$**	-
Actinides	ThF_4,UF_3, UF_4	UCl_3, UCl_4, **$PuCl_3$**	UI_3, UI_4
Pseudo-binary	53 systems (v.2) / **~70 systems (v.3)**	60 systems (v.2) / **~70 systems (v.3)**	10 systems (v.2) / **~30 systems (v.3)**
Pseudo-ternary	25 systems (v.2) / **~30 systems (v.3)**	22 systems (v.2) / **~27 systems (v.3)**	None (v.2) / **~15 systems (v.3)**

METHODOLOGY FOR GENERATING ACCURATE THERMODYNAMIC VALUES

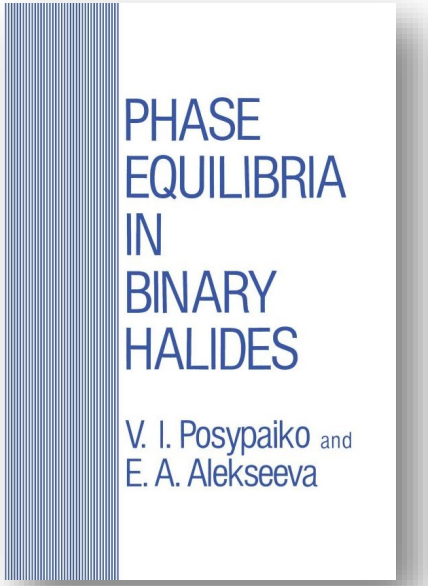
Exhaustive data mining for phase equilibria and thermodynamic data, including Non-English literature

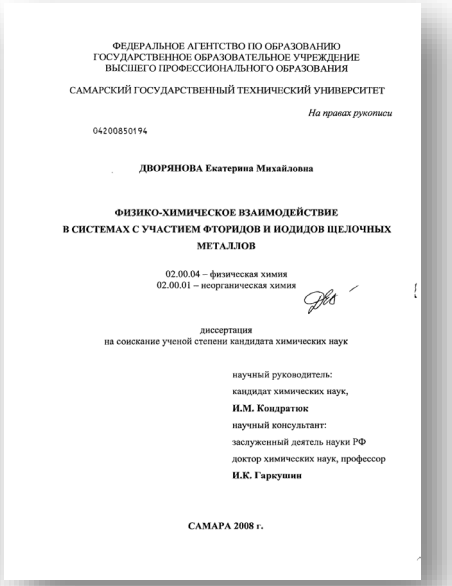
Phase equilibria



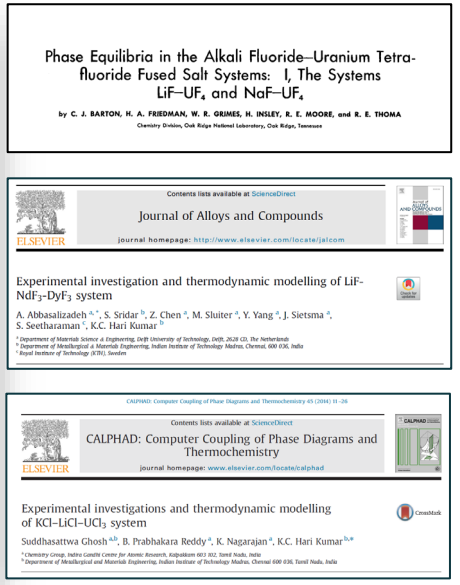
ORNL reports

Compilations





Ph.D. Thesis



Articles

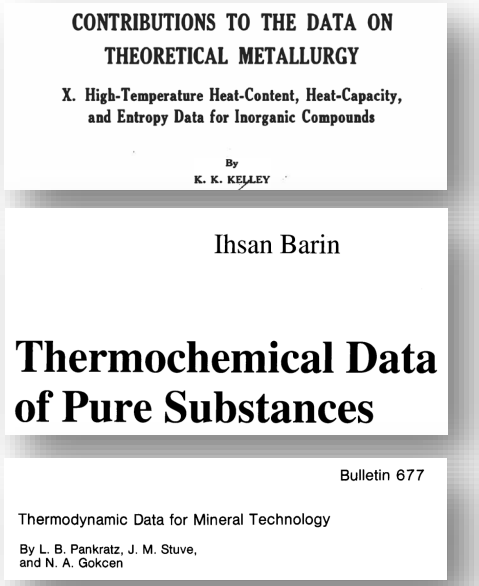
***All *MSTDB-TC* Values Traceable to Original Sources**

METHODOLOGY FOR GENERATING ACCURATE THERMODYNAMIC VALUES

Exhaustive data mining for phase equilibria and thermodynamic data, including Non-English literature

Thermodynamic properties of pure compounds

Mixtures


CONTRIBUTIONS TO THE DATA ON THEORETICAL METALLURGY

X. High-Temperature Heat-Content, Heat-Capacity, and Entropy Data for Inorganic Compounds

By K. K. KELLEY

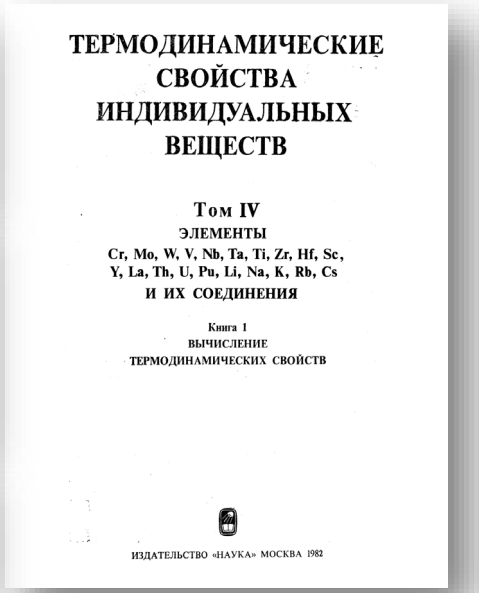
Ihsan Barin

Thermochemical Data of Pure Substances

Bulletin 677

Thermodynamic Data for Mineral Technology

By L. B. Pankratz, J. M. Stuve, and N. A. Gokcen


ТЕРМОДИНАМИЧЕСКИЕ СВОЙСТВА ИНДИВИДУАЛЬНЫХ ВЕЩЕСТВ

Том IV

ЭЛЕМЕНТЫ

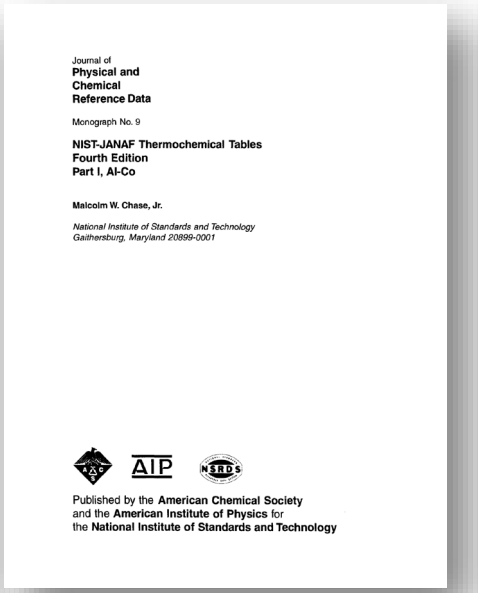
Cr, Mo, W, V, Nb, Ta, Ti, Zr, Hf, Sc, Y, La, Th, U, Pu, Li, Na, K, Rb, Cs

И ИХ СОЕДИНЕНИЯ

Книга 1

ВЫЧИСЛЕНИЕ ТЕРМОДИНАМИЧЕСКИХ СВОЙСТВ

ИЗДАТЕЛЬСТВО «НАУКА» МОСКВА 1982


Journal of Physical and Chemical Reference Data

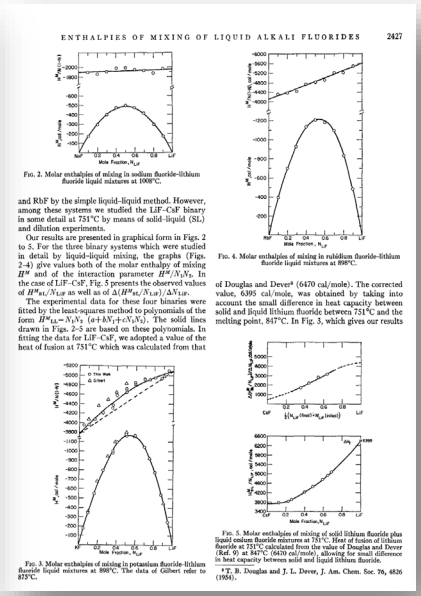
Monograph No. 9

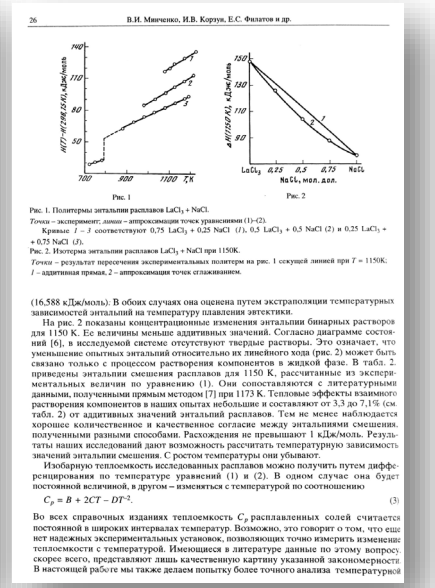
NIST-JANAF Thermochemical Tables Fourth Edition Part I, Al-Co

Malcolm W. Chase, Jr.

National Institute of Standards and Technology Gaithersburg, Maryland 20899-0001

Published by the American Chemical Society and the American Institute of Physics for the National Institute of Standards and Technology


ENTHALPIES OF MIXING OF LIQUID ALKALI FLUORIDES 2427


Compilations

Articles

***All *MSTDB-TC* Values Traceable to Original Sources**

CHALLENGES IN BUILDING A LARGE DATABASE

Stoichiometric compounds including pure salts

- Not all thermodynamic data available
- Discrepancies often observed in the tabulated thermodynamic data
- Evaluation is necessary to obtain self consistent set of Gibbs Energy parameters
- Changes in values for basic components can affect numerous systems

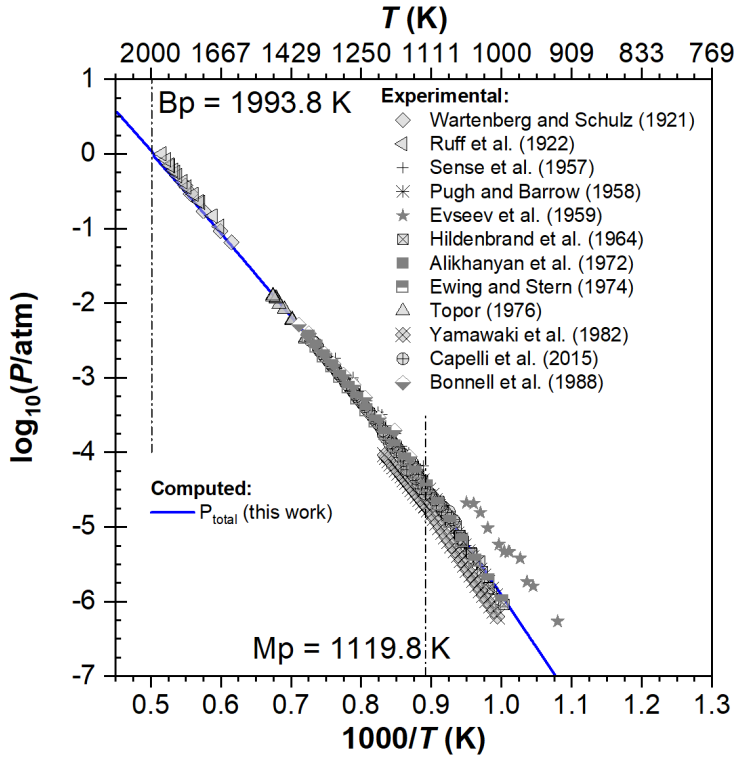
Mixed salts

- Limited data at high-temperatures for vapor pressures and excess thermodynamic properties (e.g., enthalpy of mixing)
- Few intermediate compounds have reported experimental heat capacity
- Larges discrepancies can be found in reported phase equilibria
- Listed experimental uncertainties are rarely realistic

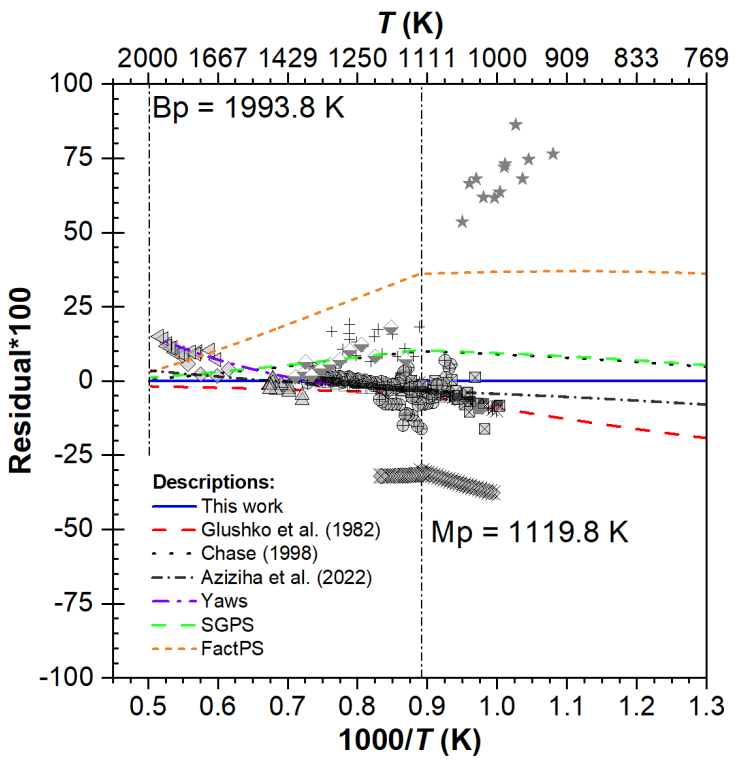
METHODOLOGY FOR GENERATING ACCURATE THERMODYNAMIC VALUES

Analysis of pure salts (gas & liquid phase)

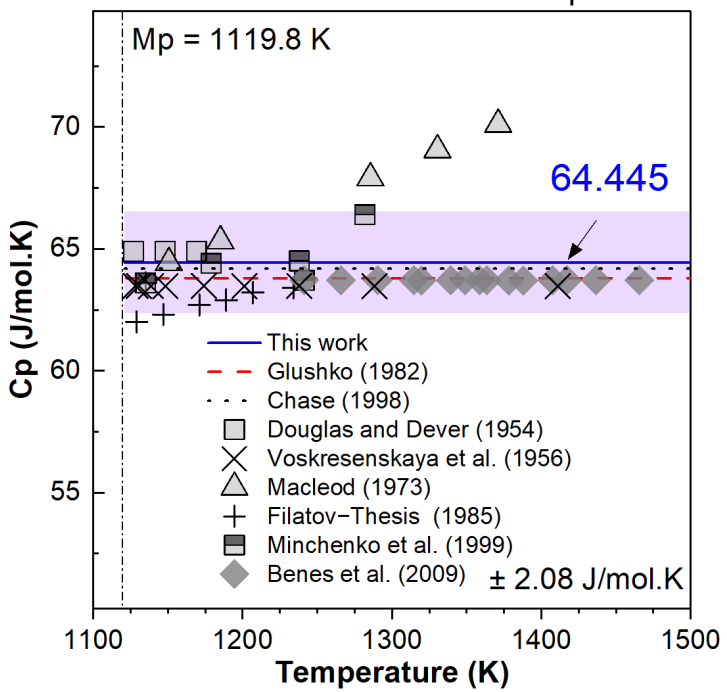
Lithium fluoride – P_{total}*



Lithium fluoride – Residual**



Lithium fluoride – C_p**



Internal work from MSTDB-TC: Same analysis for LiF, NaF, KF, BeF_2, ZrF_4, UCl_3, UCl_4, LiI, NaI, KI, CsI, BeI_2, MgI_2, UI_3, UI_4
Ongoing: NaCl, KCl, $MgCl_2$, CsCl

* Aziziha & Schorne-Pinto *et al.* (2022). *Journal of Molecular Liquids*, 364, 119973.
** Schorne-Pinto *et al.* (ongoing paper) - A Comprehensive Thermochemical Study of Liquid and Gas LiF, NaF, and KF Alkali Fluorides: How Accurate Are Their Existing Thermodynamic Functions?

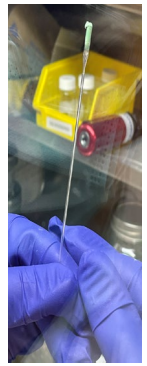
METHODOLOGY FOR GENERATING ACCURATE THERMODYNAMIC VALUES

Experimental determination of key values

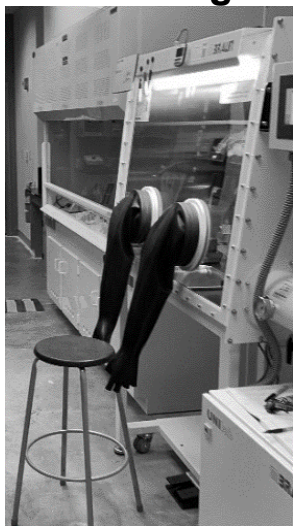
- DSC for phase transitions, ΔH_{fus} and heat capacity (up to 1200°C)
- XRD for phase identification (RT up to 1100°C)

XRD

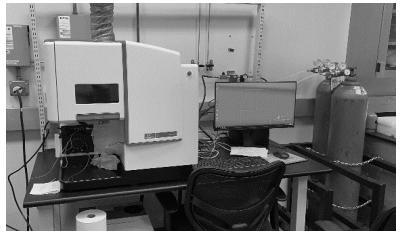
Rigaku Smartlab XRD (RT-1100 °C)



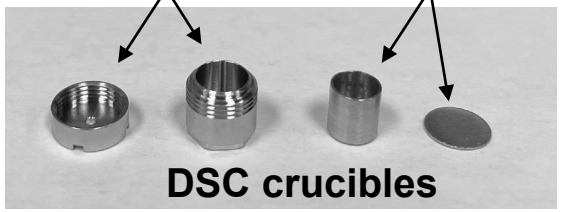
Handling



Composition: ICP-OES

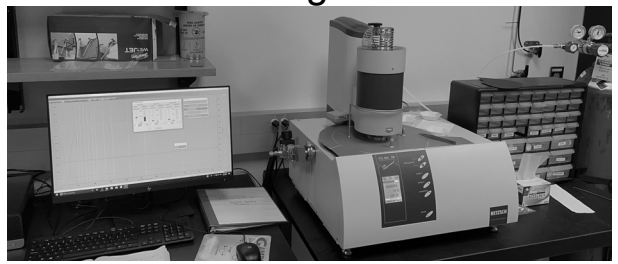


stain steel crucible/lid Ni liner and gaskets



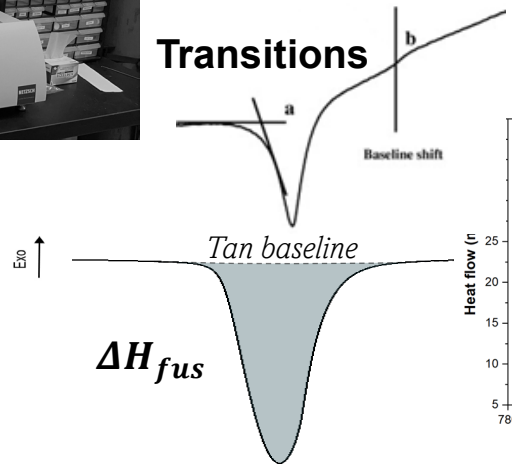
DSC crucibles

DSC 404 F3 Pegasus®

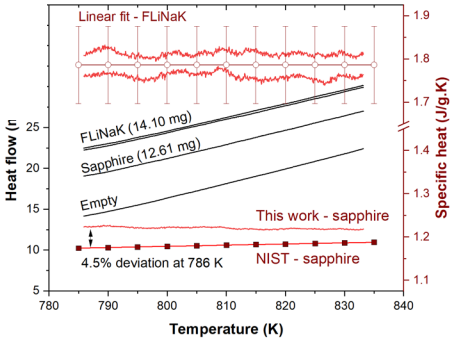


STA 449 Jupiter®

Transitions



Heat capacity



Della Gatta, G., Richardson, M. J., Sarge, S. M. & Stølen, S. (2006). *Pure and Applied Chemistry*. 78, 1455–1476

Piro, M. H. A., Lipkina, K. & Hallatt, D. (2021). *Thermochimica Acta*. 699, 178860.

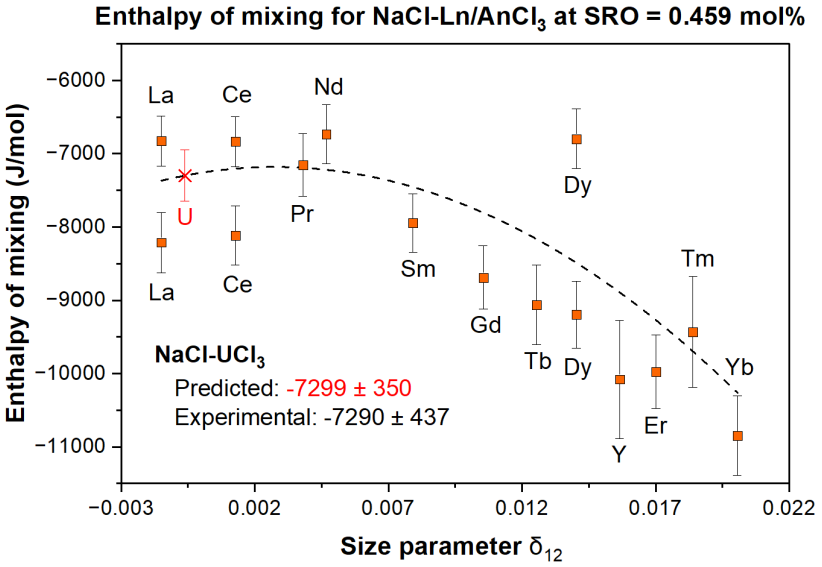
METHODOLOGY FOR GENERATING ACCURATE THERMODYNAMIC VALUES

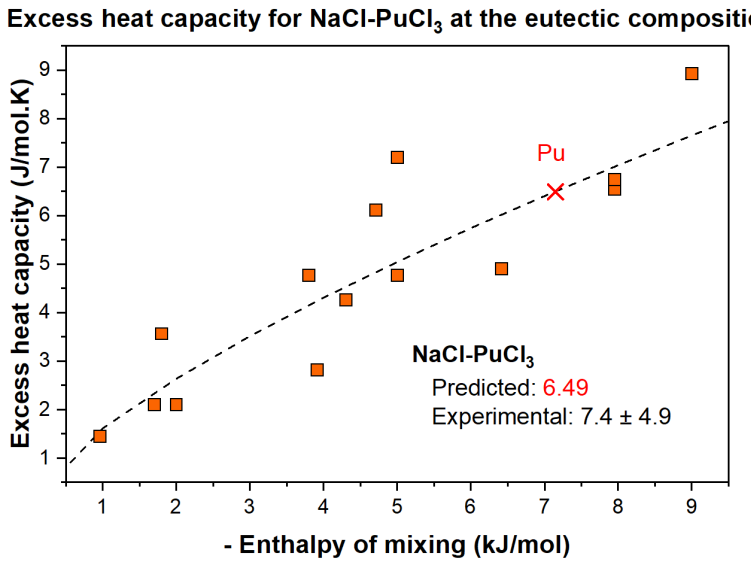
First principles calculations

- Determining energy of formation for crystalline phases
- Coordination numbers to improve molten salt models

	OQMD	MP	CALPHAD
LiF (*Fm-3m*)	-607.9	-610.9	-616.9
ZrF_4 ($P4_2/3$)	-1910.9	-1930.7	-1911.3
Li_2ZrF_6 ($P\bar{3}1m$)	-3170.4	-3196.5	-3188.8
Reaction	**-43.7**	**-44.0**	**-43.7**

Correlations to estimate enthalpy of mixing and excess heat capacity



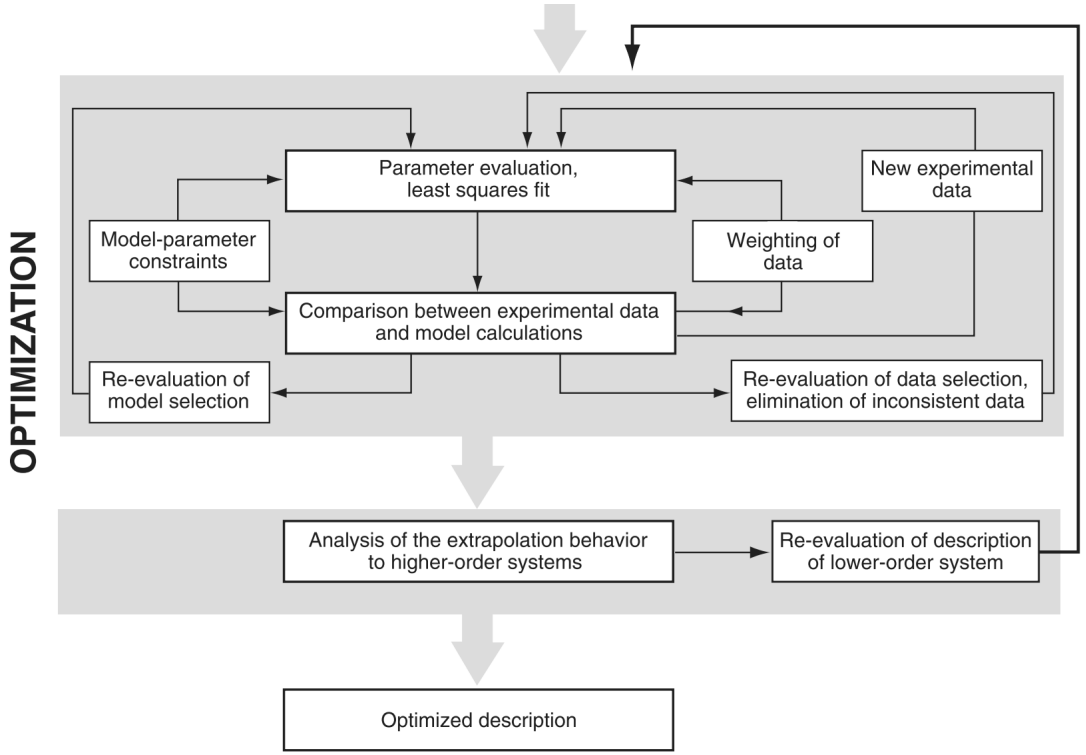


Schorne-Pinto & Yingling *et al.* (2022). ACS Omega, 7(1), 362-371.
Yingling & Schorne Pinto *et al.* (2023). *The Journal of Chemical Thermodynamics*, 179, 106974.
Matsuura et al. (2002). *J. Nucl. Sci. Technol.* 39, 632– 634.
Karlsson et al. (2022). INL/RPT-22-69181-Rev000; Idaho National Lab. (INL)

METHODOLOGY FOR GENERATING ACCURATE THERMODYNAMIC VALUES

Calphad assessments

- Assessment of all available data, including evaluation of experimental errors
- Reduced model degrees of freedom in order to prevent overfitting
- Optimization using tools or manually adjusted (depending on the system's complexity)
- Verification of the description's quality based on its capacity to reproduce phase equilibria and thermal properties
- Plot up to 5000 K to verify if any unreal immiscibility gap is formed
- High-order extrapolation for parameter validation



Schematic diagram of the Calphad assessment method, extracted from from Lukas *et al.* (2007) – *Computational Thermodynamics: The Calphad method*

CONCLUSIONS

- A thermodynamic database for molten salt applications can provide valuable information for its technical development
- Such a database is MSTDB-TC, which is now publicly available
- Gibbs energy functions/models in MSTDB-TC continue to be refined and expanded to describe relevant salt systems

ACKNOWLEDGEMENTS

U.S. Department of Energy Office of Nuclear Energy, under the Nuclear Energy Advanced Modeling and Simulation Program under subcontract CW21750 administered by the Oak Ridge National Laboratory, operated by UT-Battelle, L.L.C., for the U.S. Department of Energy under contract DE-ACO5-000R2275.

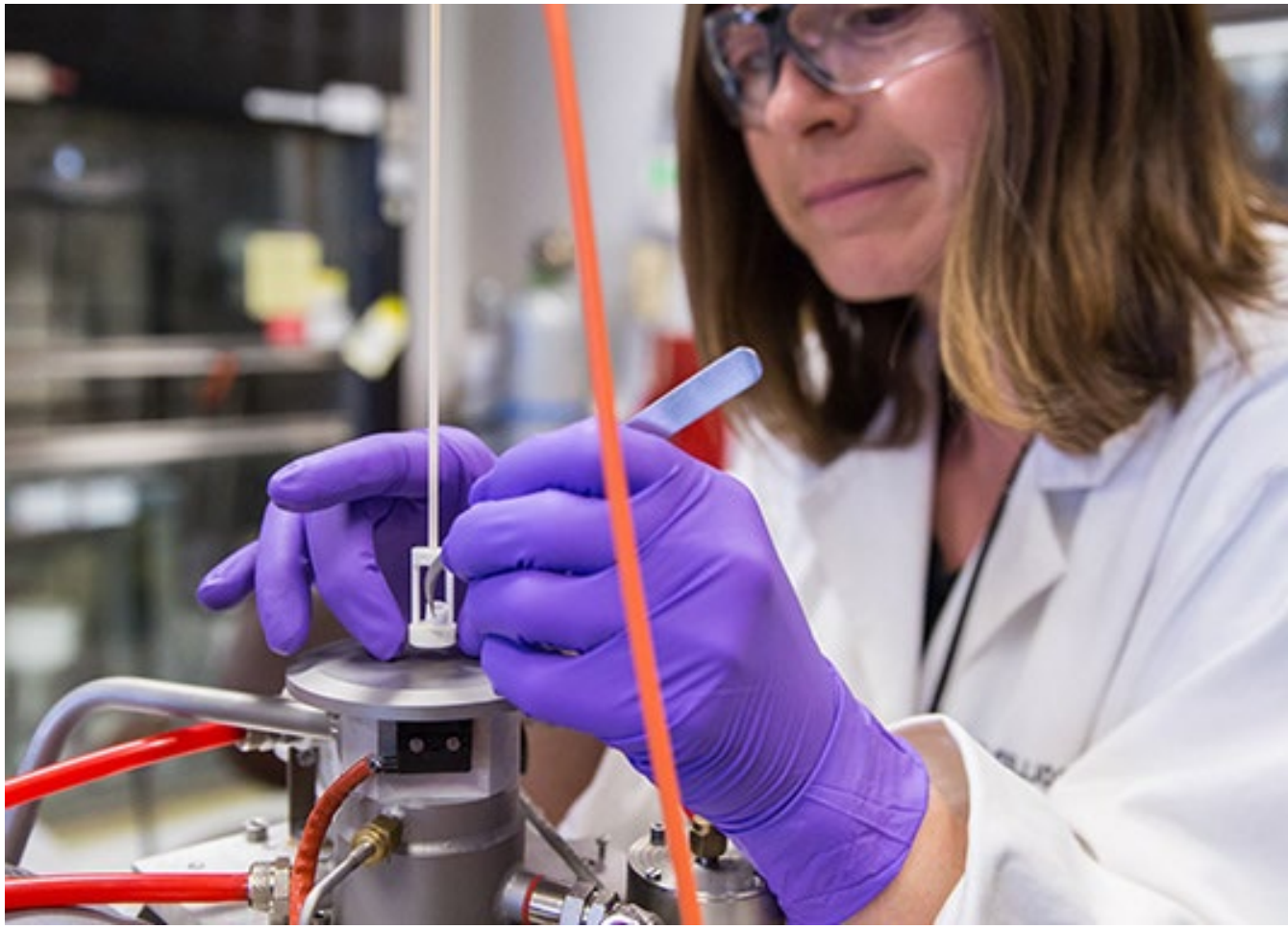
USC team

Canadian Nuclear Laboratories | Laboratoires Nucléaires Canadiens

MSTDB-TC 1.3
Quality Assessment

Max Poschmann [a,b], Markus Piro[b]
[a] Canadian Nuclear Laboratories
[b] Ontario Tech

2023 APRIL 25



Context

This work was funded by the U.S. Department of Energy's Nuclear Energy Advanced Modeling and Simulation program.

- MSTDB-TC validation available to users currently takes the form of phase diagram comparisons

1001: LiF-NaF

Fig. 1001a - Calculation saved in C:\FactSage81\ChemSage\81FwfuncV2\PD_Macro_F\BMPs\

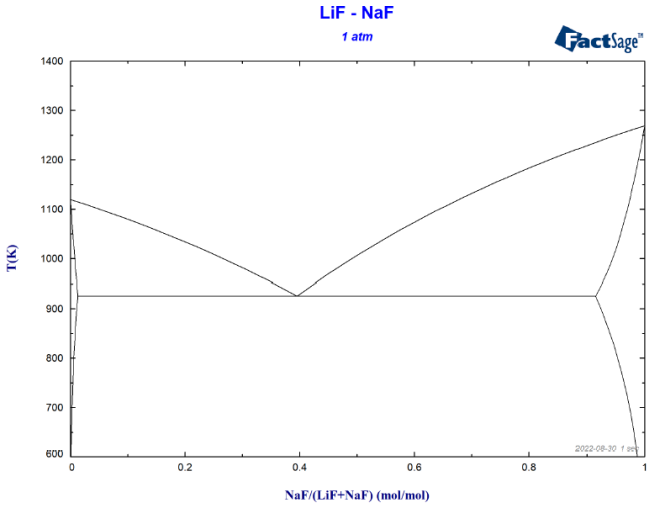
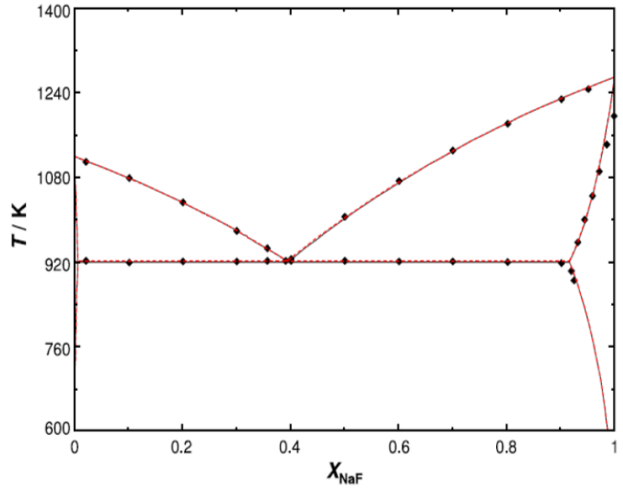


Fig. 1001b - Published figure from Ref[21] saved in C:\FactSage81\ChemSage\81FwfuncV2\PD_Macro_F\Lit
Please see Excel data package for this system for additional information.



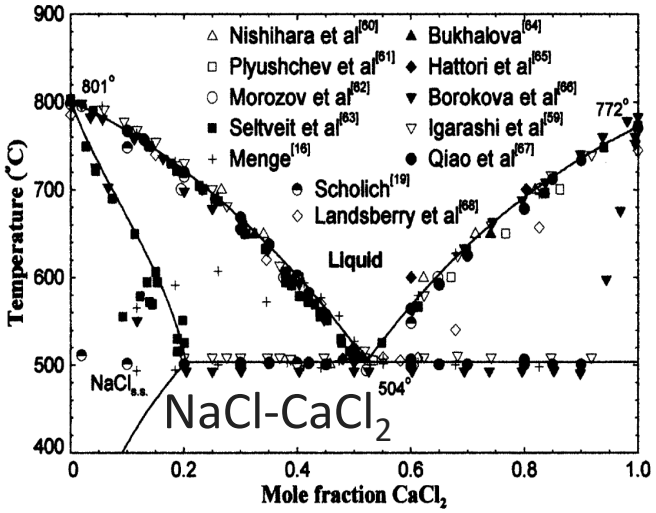
- Supplementary (independent) validation was commissioned
- Two components:
  - Qualitative assessment of available experimental data and database
  - Quantitative comparison
- Goals:
  - Provide confidence to users
  - Identify systems requiring further experimental assessment
  - Provide tools to automate validation
  - Flag issues with assessed systems
- INL/RPT-22-69782 "Development of a Gibbs Energy Minimiser for the MOOSE-based Corrosion Modelling App Yellowjacket and Validation of MSTDB" published

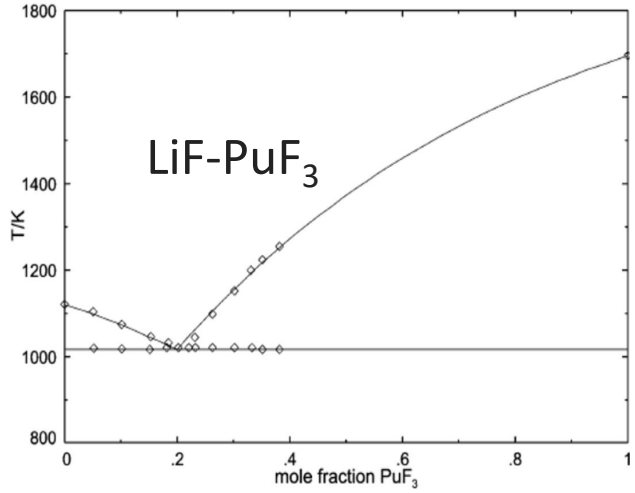
Qualitative Assessment

- Each assessed pseudo-binary subsystem was evaluated on:
  - Comprehensiveness of experimental data
  - Confidence in experimental data
- High/medium/low ratings were provided
- This evaluation identified good candidates for future experimental campaigns

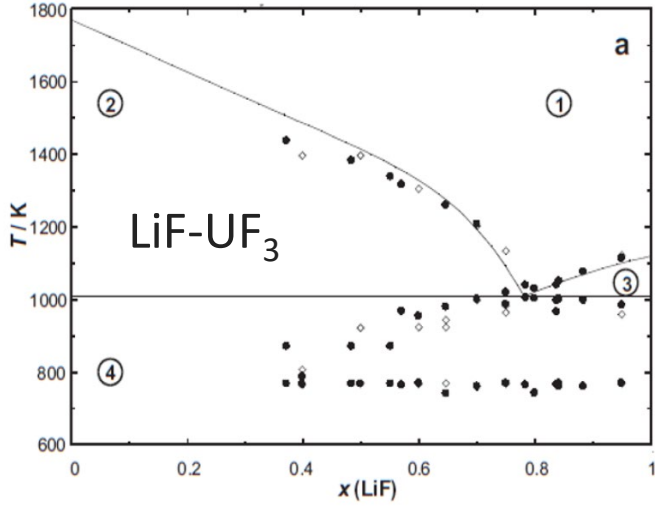
High Comprehensiveness

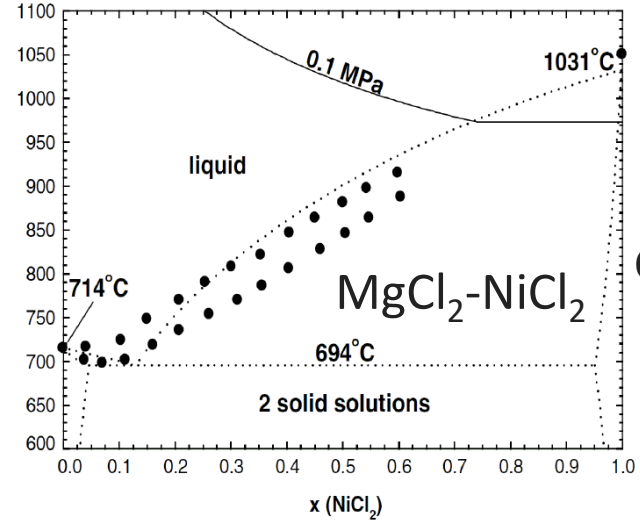
Low Comprehensiveness





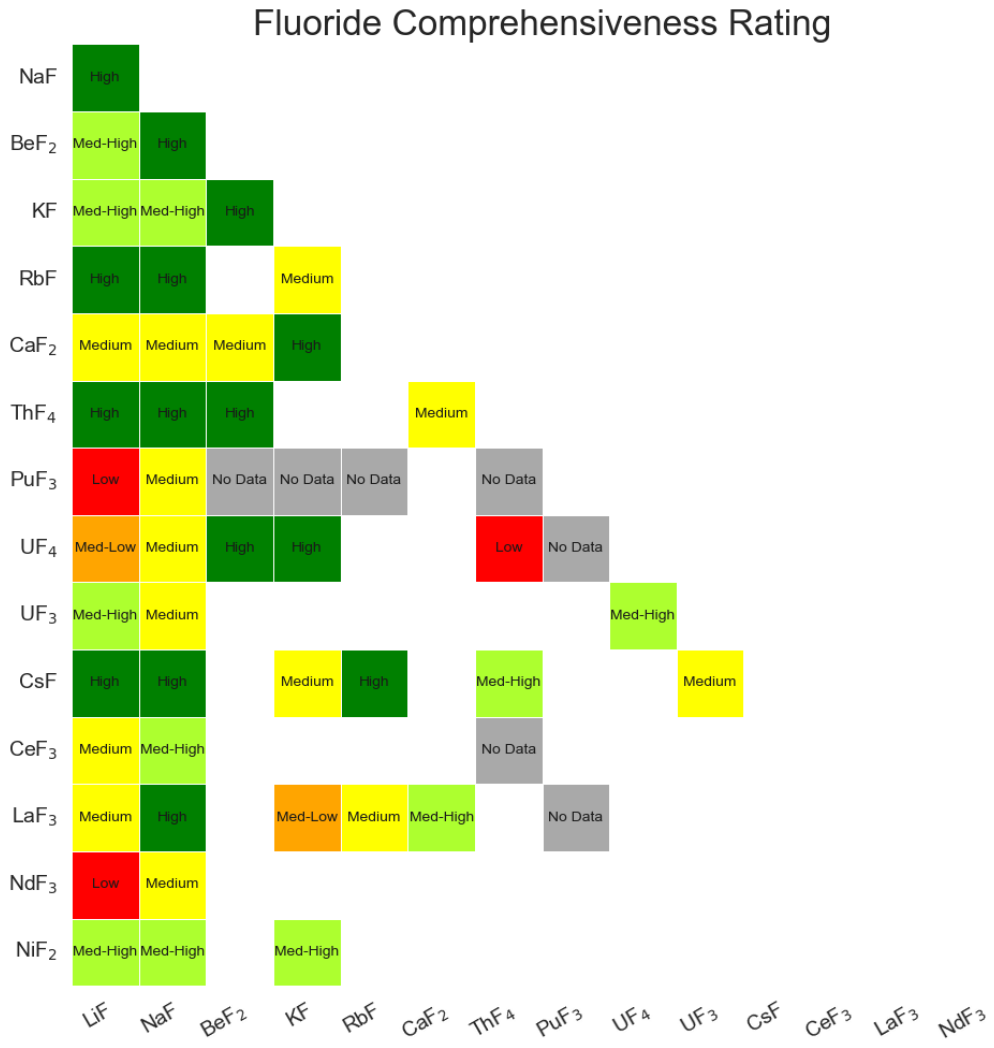
High(er) Confidence

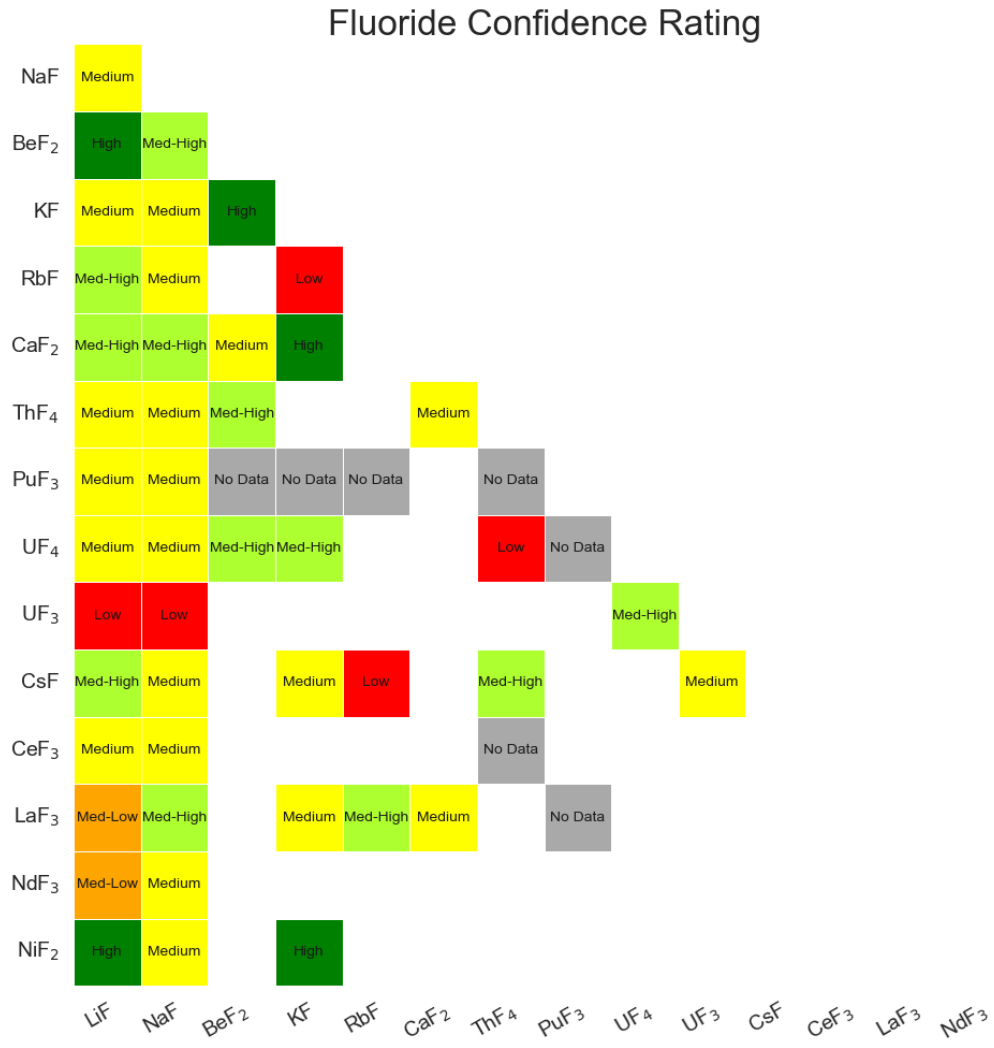




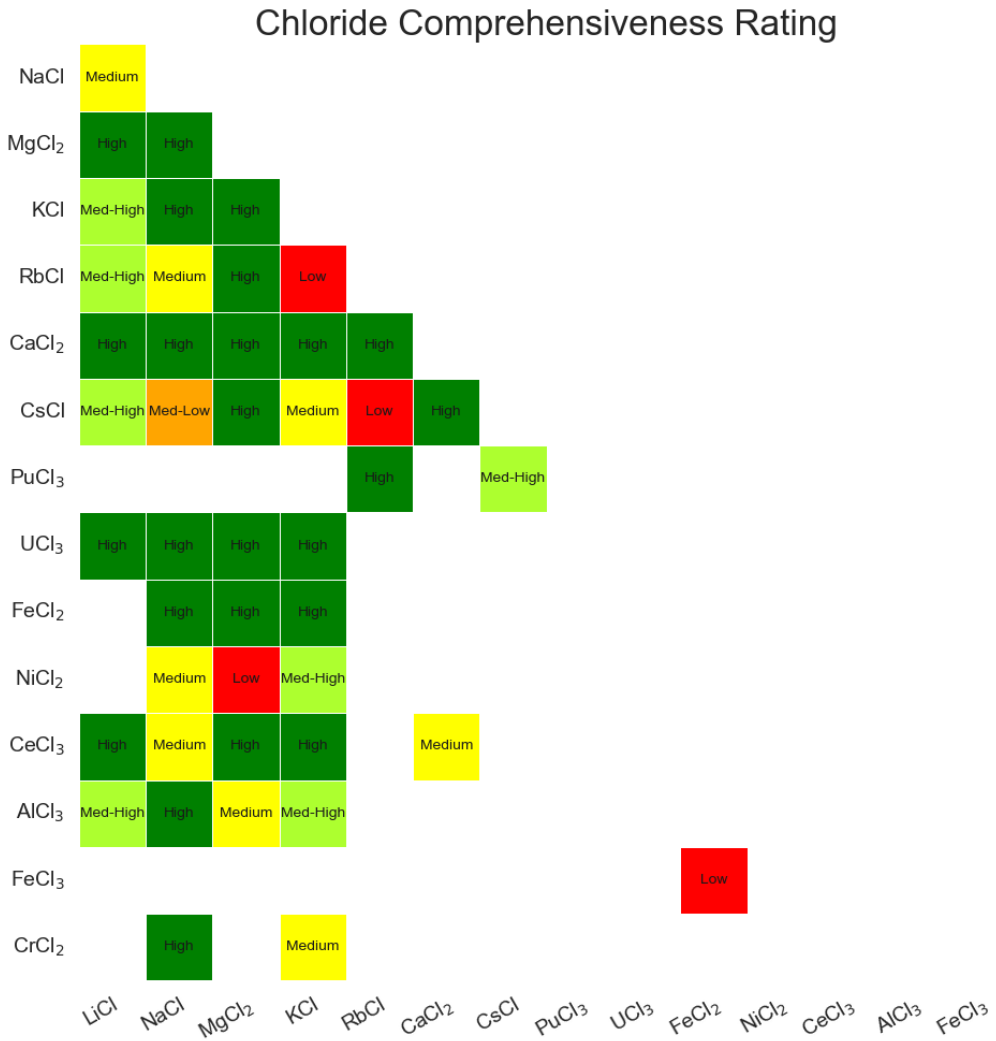
Low Confidence

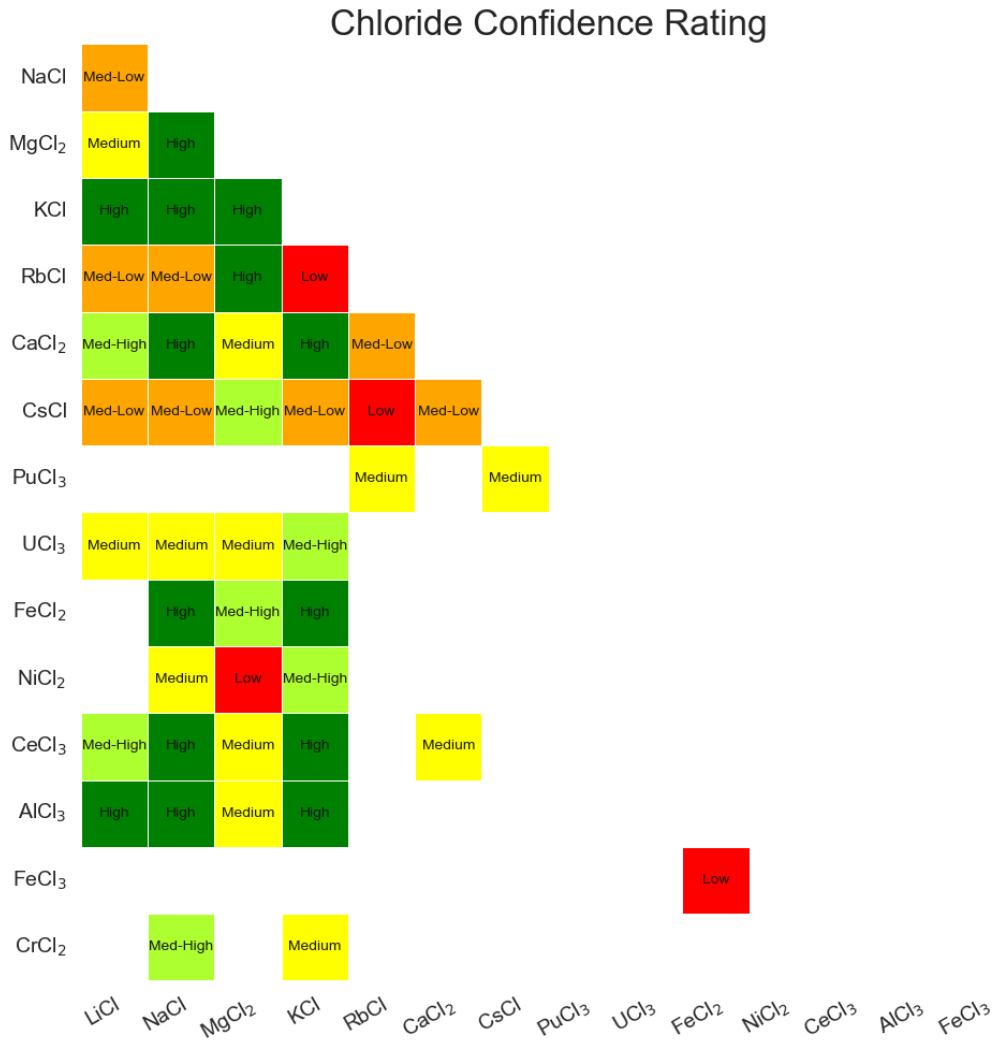
Fluoride Systems Ratings





Chloride Systems Ratings

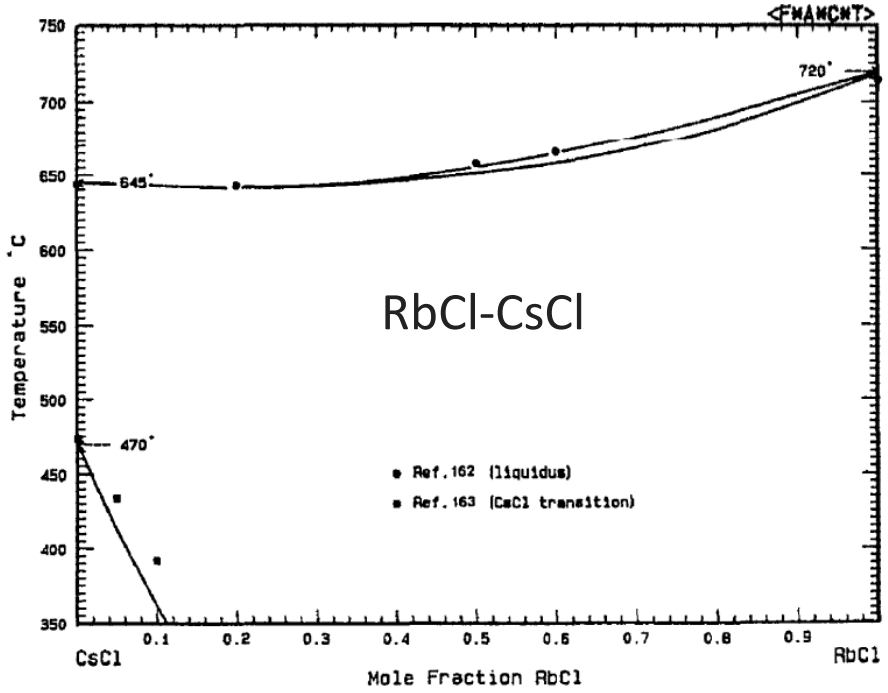




Qualitative Assessment Outcomes

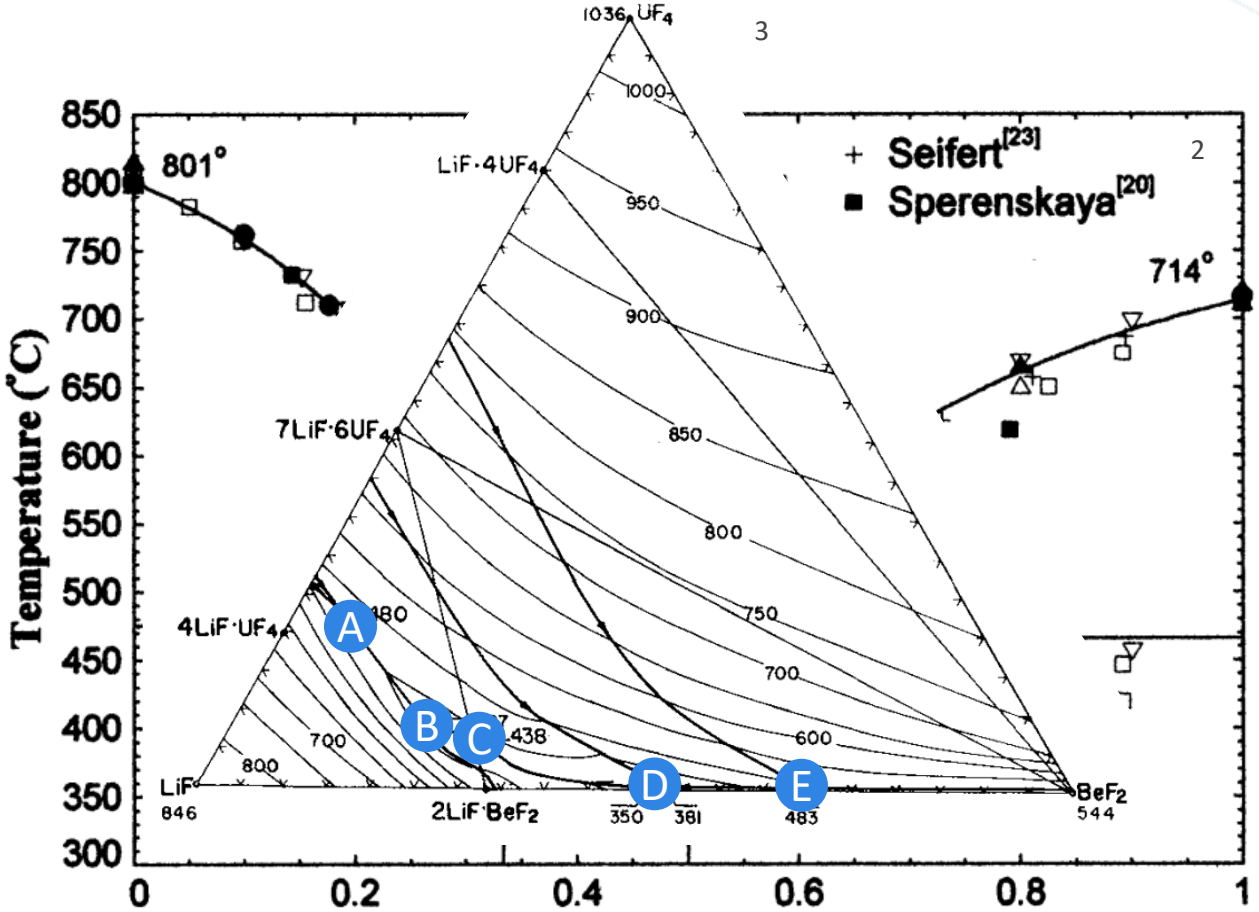
- Candidates identified for future experimental campaigns:
  - Many PuF_3 binaries are missing (BeF_2, KF) or sparsely populated (LiF)
  - Many CsCl phase diagrams with low confidence
  - Specific regions within other systems flagged, e.g. LiF-BeF_2 with x(LiF) > 0.85
- Possible additions to database:
  - Binaries: CsCl-$CeCl_3$, $CeCl_3$-RbCl, CsF-LaF_3, LiCl-$PuCl_3$, NaCl-$PuCl_3$, $CaCl_2$-$PuCl_3$
  - Ternaries: LiCl-KCl-$MgCl_2$, NaCl-KCl-$MgCl_2$

"The other four binary phase diagrams (KF–PuF_3, RbF–PuF3, CsF–PuF_3 and LaF_3–PuF_3) presented in this study have been estimated based on the data from the proxy systems containing LaF_3."
— O. Beneš and R. Konings (2008)



Quantitative Assessment

- Thermochimica used to automate comparisons between MSTDB-TC and experimental data
- Three types of experimental data points:
  - Vapor pressures
  - Solubility limits
  - Invariant transitions
- Goals:
  - Provide confidence that MSTDB-TC (with Thermochimica) is working as intended
  - Compile experimental reference data
  - Automate validation



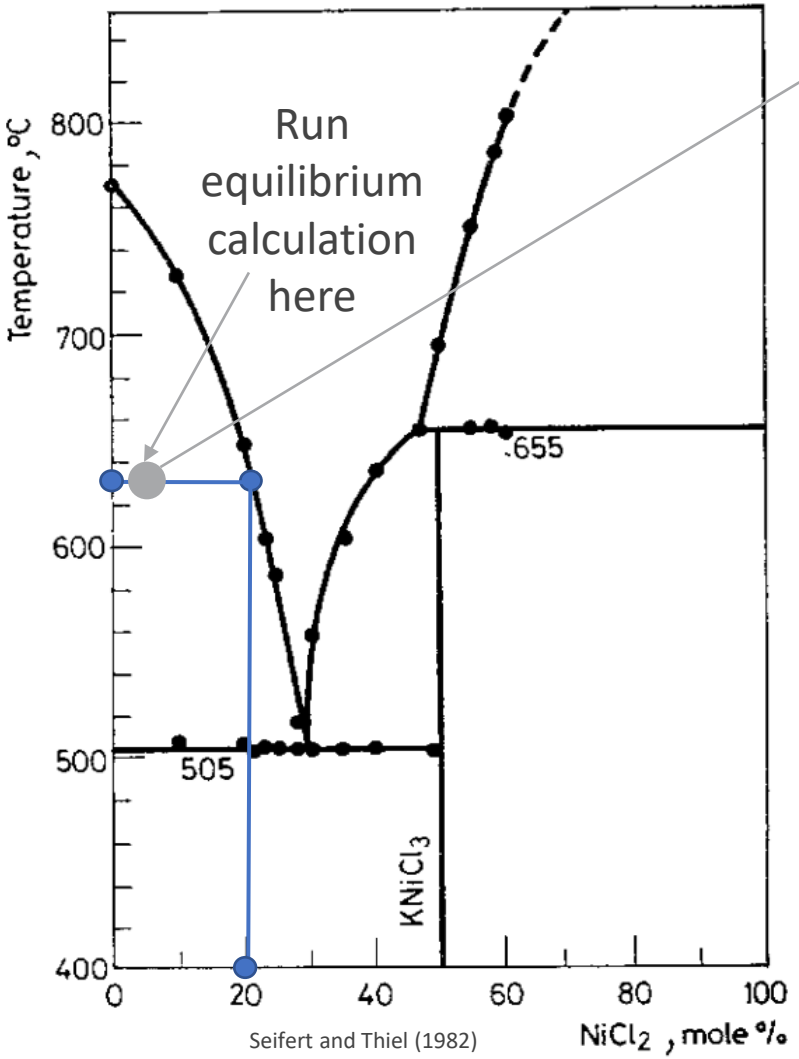
Invariant point	Invariant composition (mole %) LiF	BeF₂	UF₄	Invariant temp. (°C)	Phases present	Type of equilibrium
A	72	5.5	22.5	480	LiF–7LiF·6UF₄–4LiF·UF₄	Lower stability limit for 4LiF·UF₄
B	69.5	22.5	8	427	LiF–2LiF·BeF₂–7LiF·6UF₄	Ternary eutectic
C	65	29	6	438	2LiF·BeF₂–7LiF·6UF₄	Maximum point on boundary
D	48	51.5	0.5	350	2LiF·BeF₂–BeF₂–7LiF·6UF₄	Ternary eutectic
E	45.5	54	0.5	381	BeF₂–LiF·4UF₄–7LiF·6UF₄	Ternary peritectic
F	30.5	69	0.5	483	BeF₂–UF₄–LiF·4UF₄	Ternary peritectic

[1] Experiment: Smith, Ferris, and Thompson (1969)

[2] Pelton and Chartrand (2001)

[3] Jones *et al.* (1962)

Example Solubility Limits Test: $KCl\text{-}NiCl_2$



Seifert and Thiel (1982)

```
============================================================
|                  THERMOCHIMICA RESULTS                   |
============================================================

   0.59406 mol MSCL
Cation fractions:
                { 0.79603       K
                + 0.20397       Ni }
Anion fractions:
                { 1.00000       Cl
                + 0.00000       Va }

   0.24513 Moles of pairs
Pair fractions:
                { 0.79603       KCl
                + 1.0022E-11    K
                + 0.20397       NiCl2
                + 2.1804E-09    Ni    }

Quadruplet fractions:
                { 0.50958       K-K-Cl-Cl
                + 1.4578E-02    Ni-Ni-Cl-Cl
                + 0.47584       K-Ni-Cl-Cl
                + 1.0133E-26    K-K-Va-Va
                + 4.9657E-16    Ni-Ni-Va-Va
                + 4.4863E-21    K-Ni-Va-Va
                + 1.4371E-13    K-K-Cl-Va
                + 5.3812E-09    Ni-Ni-Cl-Va
                + 3.6434E-11    K-Ni-Cl-Va }

 + 0.75487 mol KCl_Sylvite(s)
```

Check $NiCl_2$ concentration of liquid at equilibrium

Check solid and liquid phases are present

Test Database and Automation

- Experimental data compiled (with metadata) in JSON test database
- Python scripts to:
  - Read experiments from test database
  - Run tests in Thermochimica
  - Compare results
  - Update JSON with test results
- Can query/run tests based on:
  - Publication ID
  - Test status
  - Constituent elements
- Most tests run in <1 second


```
"seifert-1982": {
  "mstdb references": [
    "mstdb-40:robelin2004"
  ],
  "url": "https://link.springer.com/article/10.1007/BF01912954",
  "title": "Thermal analysis by EMF-measurements on solid electrolytes",
  "authors": "H. J. Seifert and G. Thiel",
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            }
```
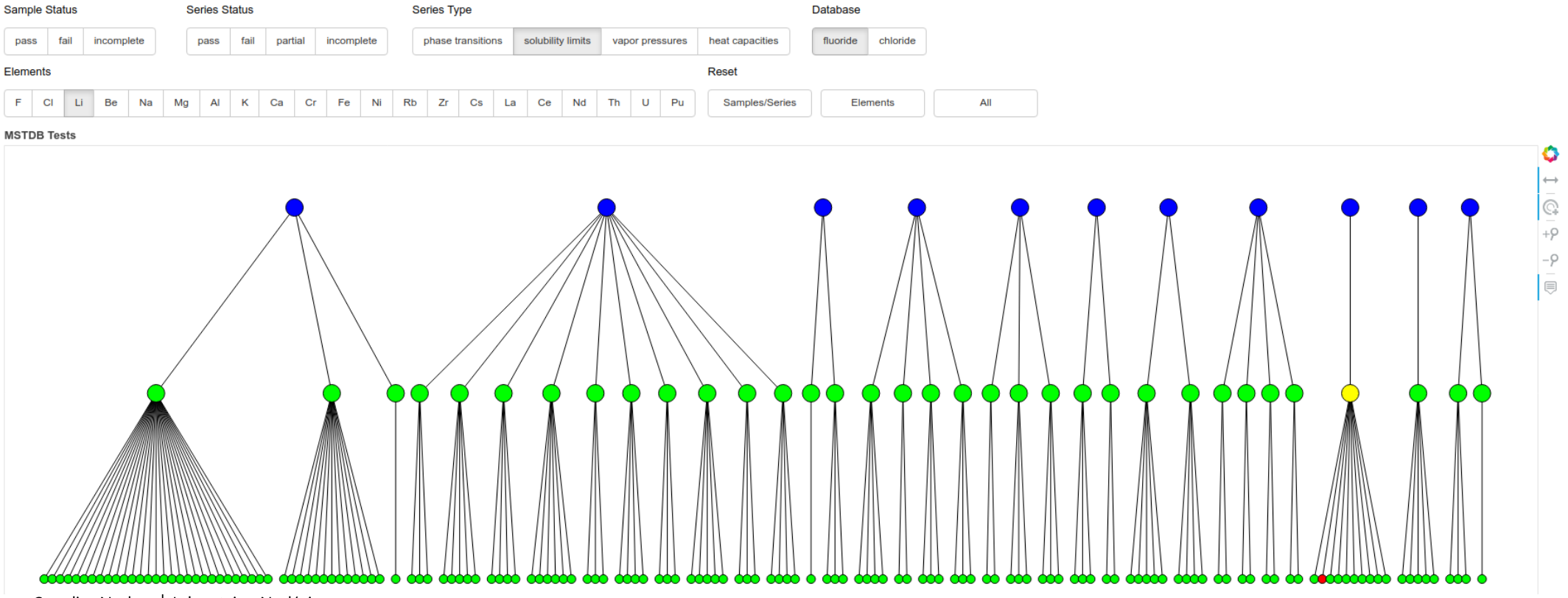

Current Status

- 1168 validation tests from 88 experimental sources have been compiled
- 47 pseudobinary fluorides, 42 pseudobinary chlorides,
  24 pseudoternary fluorides, and 10 pseudoternary chlorides tested
- Liquid-focused: all tests involve either MSFL or MSCL liquid phases
- Interactive dashboard to view validation results has been created



Quantitative Assessment Outcomes

- MSTDB-TC v1.3 shown to match experimental data within tolerance in vast majority of test cases
- Convergence issues for small group of stoichiometric chloride salts identified

*Note: it is neither possible nor desirable to match **every** available experimental datapoint.*

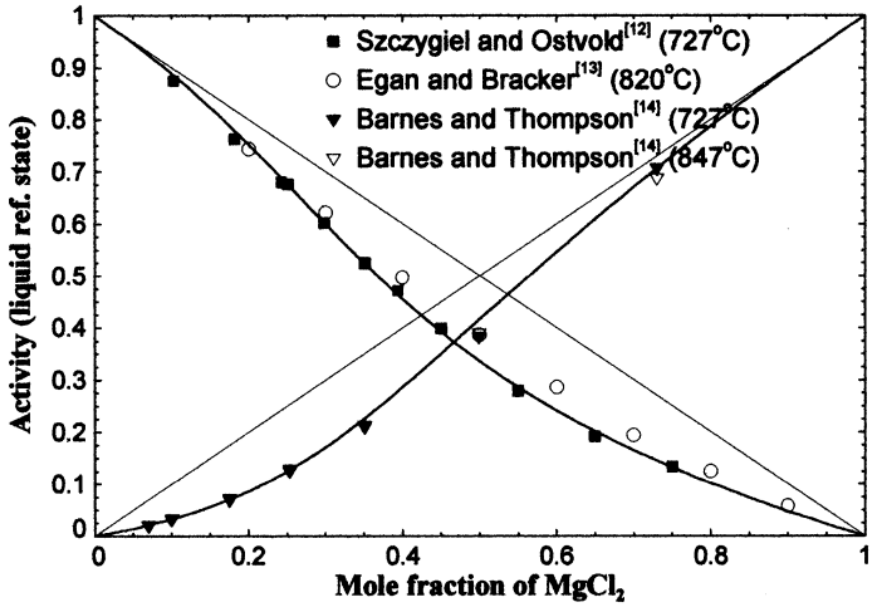
Table 3: Status of quantitative validation for ternary fluoride subsystems included in MSTDB-TC V1.3.

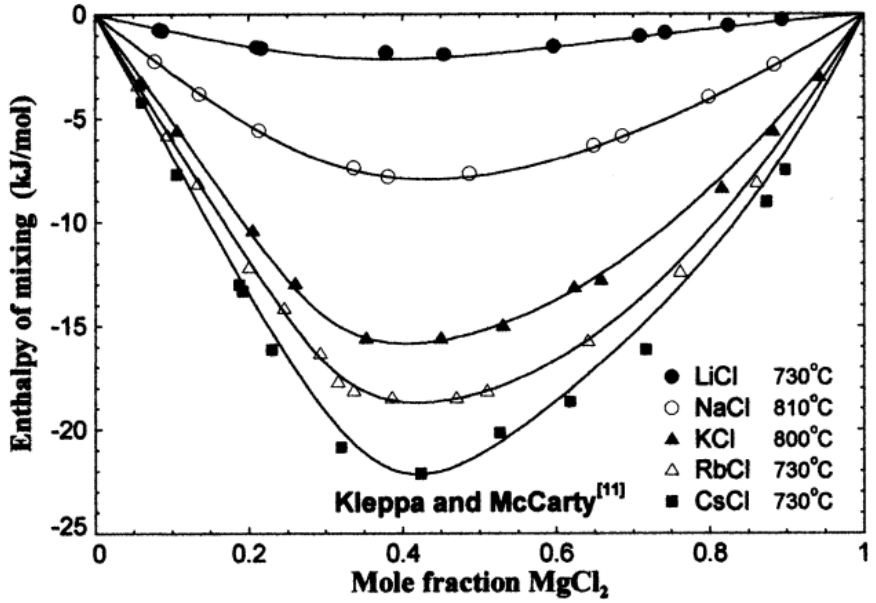
Subsystem	Invariant Transitions	Solubility Limits	Vapor Pressures	References
BeF - LiF - PuF_3		40/40		[16]
BeF - LiF - ThF_4	6/6	5/5	4/6	[11, 16, 24]
BeF - LiF - UF_4	10/11		7/7	[11, 23, 24]
BeF - NaF - PuF_3		20/20		[16]
BeF - NaF - UF_4	2/3			[37]
BeF - ThF_4 - UF_4	6/6			[24]
CaF_2 - KF - LiF	1/2			[26]
CaF_2 - KF - NaF	2/2			[38]
CaF_2 - LaF_3 - LiF	6/6			[18]
CaF_2 - LaF_3 - NaF	6/6			[18]
CaF_2 - LiF - ThF_4	0/1			[29]
CeF_3 - LiF - NaF	2/2			[22]
CeF_3 - LiF - ThF_4		8/8		[31]
CsF - KF - LiF	1/2			[27]
KF - LiF - NaF	1/1			[21]
KF - LiF - RbF	0/1			[15] See note (a)
LiF - NaF - LaF_3	3/3			[18]
LiF - NaF - PuF_3		7/7		[16]
LiF - NaF - RbF	1/1			[15]
LiF - NaF - ThF_4	2/3			[20]
LiF - NaF - UF_4	1/3			[19]
LiF - PuF_3 - ThF_4		5/5		[16]
LiF - PuF_3 - UF_4				See note (b)
LiF - ThF_4 - UF_4	6/6			[24]
NaF - ThF_4 - UF_4	0/4			[13]

Notes: (a) MSTDB-TC references [53], which states "the peritectic invariant point was not observed", and thus it is not included in the assessment. However, this is the only available experimental data point suitable for evaluation in the current validation scheme. (b) LiF-PuF_3-UF_4: MSTDB-TC references [55]. LiF-PuF_3-UF_4 is absent from the experimental reference Table 3. No experimental data points are plotted in figures either. The descriptions of the experimental references make no mention of this subsystem. Possibly fit entirely by using other systems as analogs.

Quantitative Assessment: Recommended Future Work

- New test classes could leverage existing experimental data:
  - Chemical potential/emf
  - Enthalpy/entropy of mixing
- Expand tests on higher-order systems
  - Comparisons to experiment
  - Consistency checks
- Dashboard release to users
  - Allow users to specify tolerances





Pelton and Chartrand (2001)

Thermodynamic Source Experimental/ Ab-initio Database (TSEAD)

- OECD/NEA collaboration intended to compile and curate available thermodynamic reference data
- Relational database format
- Intended to assist:
  - Accessibility of data (searchable)
  - Thermodynamic database optimization/re-optimization
  - Validation
  - Quality assurance
    - Tracking of data origins
    - Uncertainty quantification
  - Future applications
- Contact max.poschmann@cnl.ca

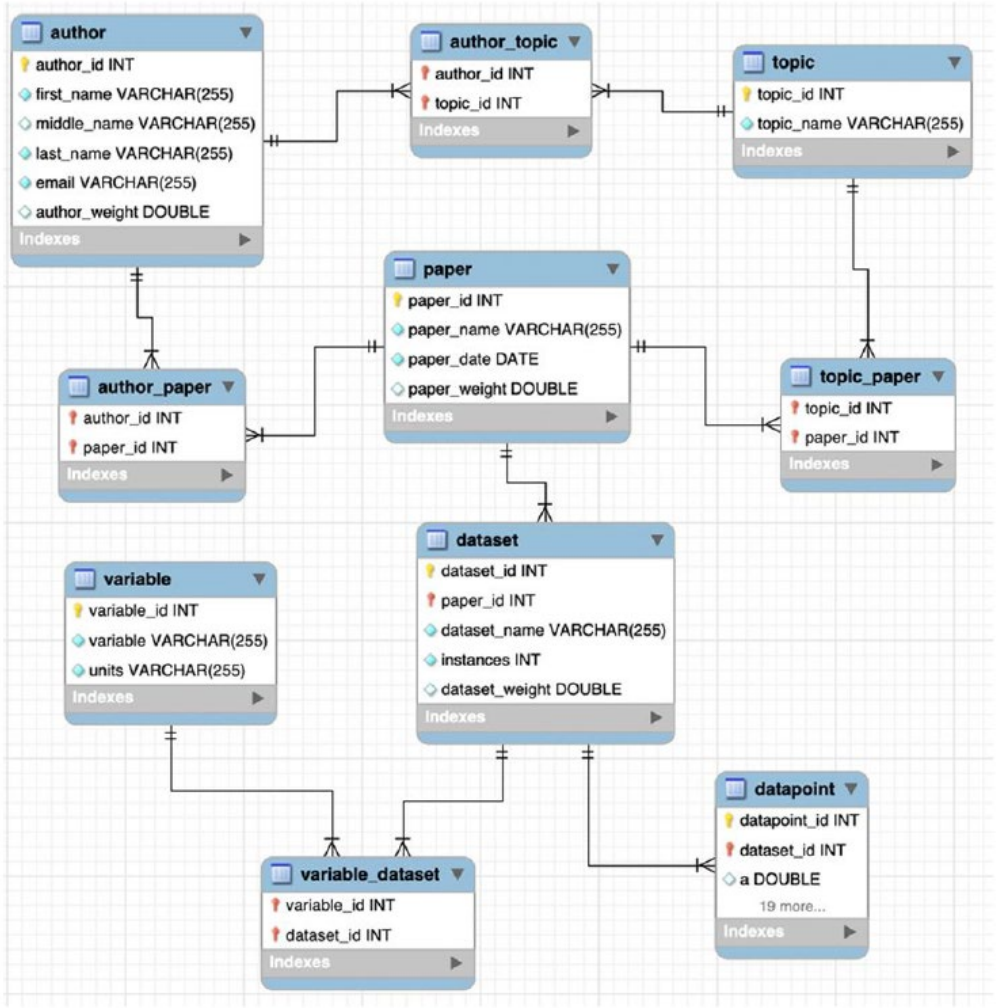
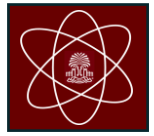


Figure 6: Schematic relational database structure.

Thank you.



General Atomics SmartState Center for Transformational Nuclear Technologies

Using MSTDB-TC with FactSage and Examples

Ted Besmann
University of South Carolina

NEUP Nuclear Energy University Program
U.S. Department of Energy

UNIVERSITY OF South Carolina

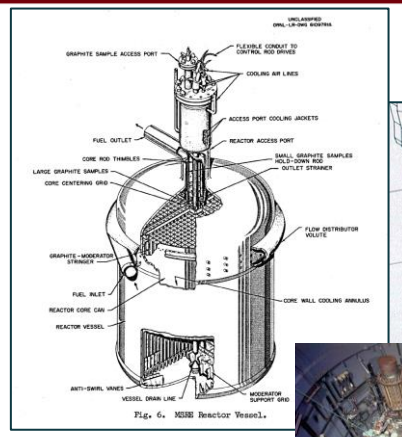
NEAMS
Nuclear Energy Advanced Modeling and Simulation

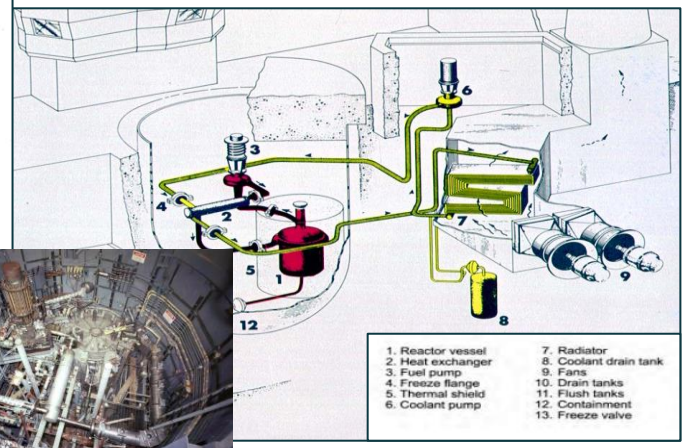
Molten Salt Reactor PROGRAM

Contents

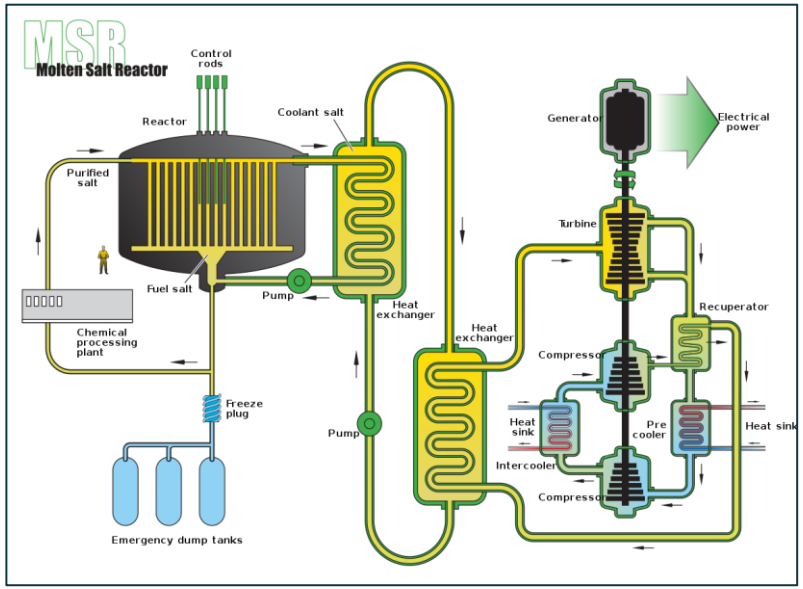
- Accessing MSTDB-TC
- Applicable FactSage modules/capabilities
- Installing database/conversion to internal format
- Caveats in application of MSTDB-TC models
- Examples
  - Computing phase equilibria and species concentrations
  - Drawing liquidus projections
  - Vapor pressure calculations
  - Corrosion product concentrations from salt equilibration with alloy
  - Salt behavior during burnup – computing change in liquidus temperature

Molten Salt Reactor Experiment 1965-71





The Future?



MSTDB-TC and -*TP* Available via DOE GitLab Site

- 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

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).

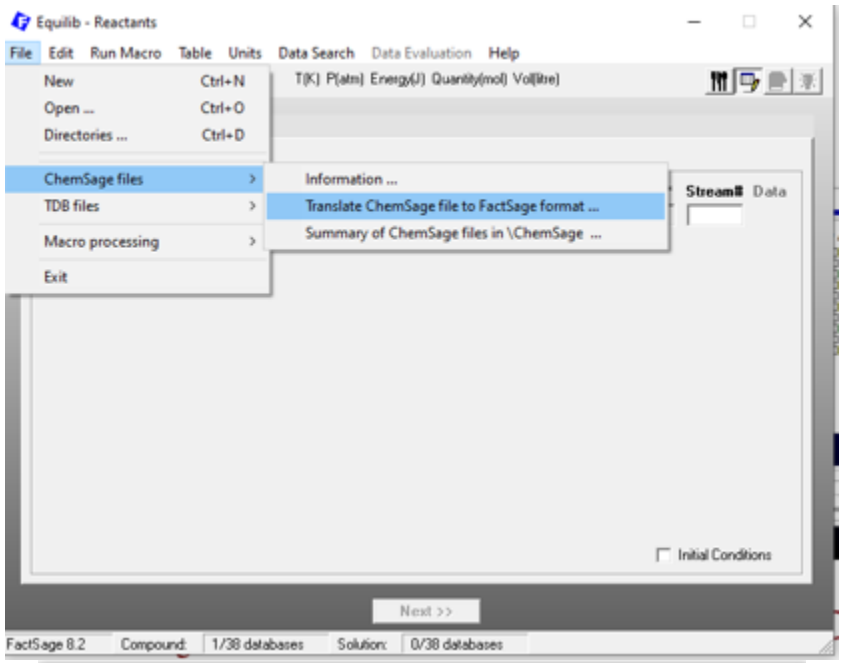
The models and values provided within MSTDB will be obtained through combinations of literature-reported information, first principles calculations, and experimental measurements. These will be used to a greater or lesser extent as needed in assessments for binary, ternary, and higher order systems. 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.

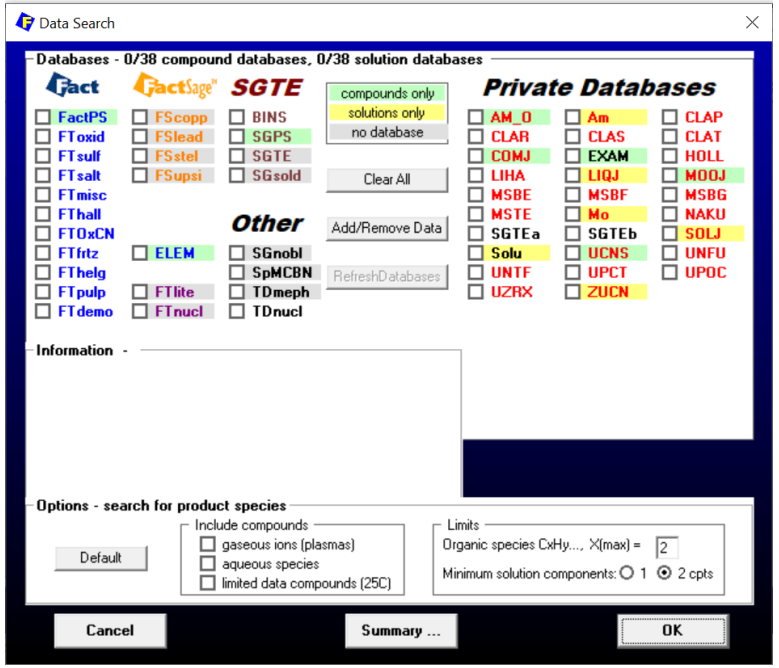
MSTDB-TC Databases Use With FactSage Allow Performance of a Variety of Calculations

- Modules can compute
  - Specific reaction energetics
  - Predominance diagrams
  - Complex, multicomponent equilibria (including vapor pressures)
  - Binary and ternary phase diagrams including
    - Liquidus and solidus projections
    - Isopleths for higher order systems
  - Additional databases can be used together to model behavior with
    - Structural alloy (corrosion)
    - Noble metal alloy
    - Other

Installing MSTDB-TC Ver. 2 Files in FactSage

- Download ASC II (.dat) files from GitHub
-
- Install using FactSage “Equilib” module
  - Fluorides: MSBF.dat generates
    - FactSage format elements/compounds files: MSBFBASE.xx
    - FactSage format for solutions files: MSBFsoln.yyy
  - Chlorides: MSTE.dat generates
    - FactSage format elements/compounds file: MSTEBASE.xxx
    - FactSage format for solutions: MSTEsoln.yyy
- Follow directions in FactSage to add a database to the library of available databases





MSTDB-TC Ver. 2.0 Assessed Systems

Pseudo-binary Systems

Fluorides

BeF_2-CaF_2
BeF_2-KF
BeF_2-LiF
BeF_2-NaF
BeF_2-PuF_3
BeF_2-ThF_4
BeF_2-UF_4
CaF_2-KF
CaF_2-LaF_3
CaF_2-LiF
CaF_2-NaF
CaF_2-ThF_4
CeF_3-LiF
CeF_3-NaF
CeF_3-ThF_4
CsF-CsI
CsF-KF
CsF-LiF
CsF-NaF
CsF-RbF
CsF-ThF_4
CsF-UF_3
CsF-UF_4
KF-KI
KF-LaF_3
KF-LiF
KF-NaF
KF-NiF_2
KF-RbF
KF-UF_4
LaF_3-LiF
LaF_3-NaF
LaF_3-RbF
LiF-LiI
LiF-NaF
LiF-NdF_3
LiF-NiF_2
LiF-PuF_3
LiF-RbF
LiF-ThF_4
LiF-UF_3
LiF-UF_4
NaF-NaI
NaF-NdF_3
NaF-NiF_2
NaF-RbF
NaF-ThF_4
NaF-UF_3
NaF-UF_4
PuF_3-ThF_4
PuF_3-UF_4
ThF_4-UF_4
UF_3-UF_4

Chlorides

$AlCl_3$-KCl
$AlCl_3$-LiCl
$AlCl_3$-$MgCl_2$
$AlCl_3$-NaCl
$CaCl_2$-$CeCl_3$
$CaCl_2$-CsCl
$CaCl_2$-KCl
$CaCl_2$-LiCl
$CaCl_2$-$MgCl_2$
$CaCl_2$-NaCl
$CaCl_2$-RbCl
$CeCl_3$-KCl
$CeCl_3$-LiCl
$CeCl_3$-$MgCl_2$
$CeCl_3$-NaCl
$CrCl_2$-KCl
$CrCl_2$-$MgCl_2$
$CrCl_2$-NaCl
$CrCl_2$-UCl_3
$CrCl_3$-KCl
$CrCl_3$-$MgCl_2$
$CrCl_3$-NaCl
CsCl-CsI
CsCl-KCl
CsCl-LiCl
CsCl-NaCl
CsCl-$PuCl_3$
CsCl-RbCl
$FeCl_2$-$FeCl_3$
$FeCl_2$-KCl
$FeCl_2$-$MgCl_2$
$FeCl_2$-NaCl
$FeCl_2$-$NiCl_2$
KCl-KI
KCl-LiCl
KCl-$MgCl_2$
KCl-NaCl
KCl-$NiCl_2$
KCl-RbCl
KCl-UCl_3
KCl-UCl_4
K-KCl
LiCl-LiI
LiCl-$MgCl_2$
LiCl-NaCl

Pseudo-ternary Systems

Fluorides

BeF_2-LiF-PuF_3
BeF_2-LiF-ThF_4
BeF_2-LiF-UF_4
BeF_2-NaF-PuF_3
BeF_2-ThF_4-UF_4
CaF_2-KF-LiF
CaF_2-KF-NaF
CaF_2-LaF_3-LiF
CaF_2-LaF_3-NaF
CaF_2-LiF-ThF_4
CeF_3-LiF-NaF
CeF_3-LiF-ThF_4
CsF-KF-LiF
CsF-KF-NaF
KF-LiF-NaF
KF-LiF-RbF
LaF_3-LiF-NaF
LiF-NaF-PuF_3
LiF-NaF-RbF
LiF-NaF-ThF_4
LiF-NaF-UF_4
LiF-PuF_3-ThF_4
LiF-PuF_3-UF_4
LiF-ThF_4-UF_4
NaF-ThF_4-UF_4

Chlorides

$AlCl_3$-KCl-LiCl
$AlCl_3$-KCl-NaCl
$AlCl_3$-LiCl-NaCl
$CaCl_2$-$CeCl_3$-LiCl
$CaCl_2$-$CeCl_3$-$MgCl_2$
$CaCl_2$-$CeCl_3$-NaCl
$CeCl_3$-KCl-LiCl
$CeCl_3$-KCl-$MgCl_2$
$CeCl_3$-KCl-NaCl
$CeCl_3$-LiCl-$MgCl_2$
$CrCl_2$-KCl-$MgCl_2$
$CrCl_2$-KCl-NaCl
$CrCl_2$-$MgCl_2$-NaCl
$FeCl_2$-KCl-NaCl
$FeCl_2$-$MgCl_2$-NaCl
KCl-LiCl-NaCl
KCl-LiCl-UCl_3
KCl-$MgCl_2$-NaCl
KCl-$MgCl_2$-$NiCl_2$
KCl-NaCl-$NiCl_2$
KCl-NaCl-UCl_3
KCl-NaCl-UCl_4

Higher Order Systems

BeF_2-LiF-ThF_4-UF_4
LiF-NaF-ThF_4-UF_4
$AlCl_3$-KCl-LiCl-NaCl
$CeCl_3$-KCl-LiCl-NaCl
$CrCl_2$-KCl-$MgCl_2$-NaCl

Caveats on Computing Equilibria in Melt

- *Calculations can be performed for any combination of components, however accuracy is not assured if the system is not listed as assessed*
- *Regardless, results of calculations for components not assessed together are expected to be sufficiently accurate*
  - *Major components have been assessed together (next release more complete)*
  - *Interactions among dilute concentration components will not be significant*
- *Individual halide component heat capacities are accurate, however, computed heat capacities for mixtures may not be accurate due to temperature dependence formalism – Utilize MSTDB-TP for complex system values*

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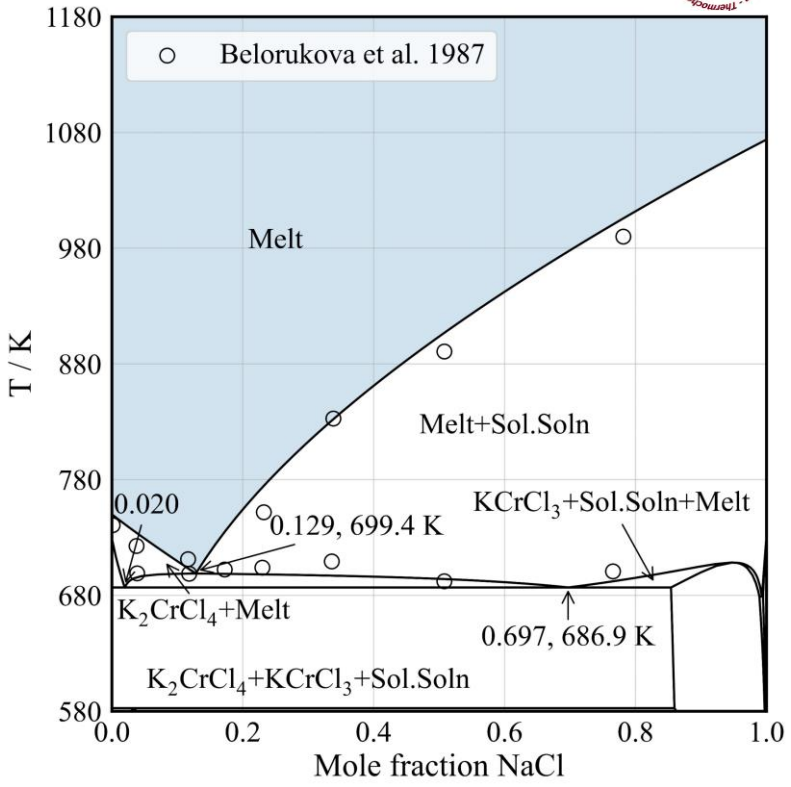
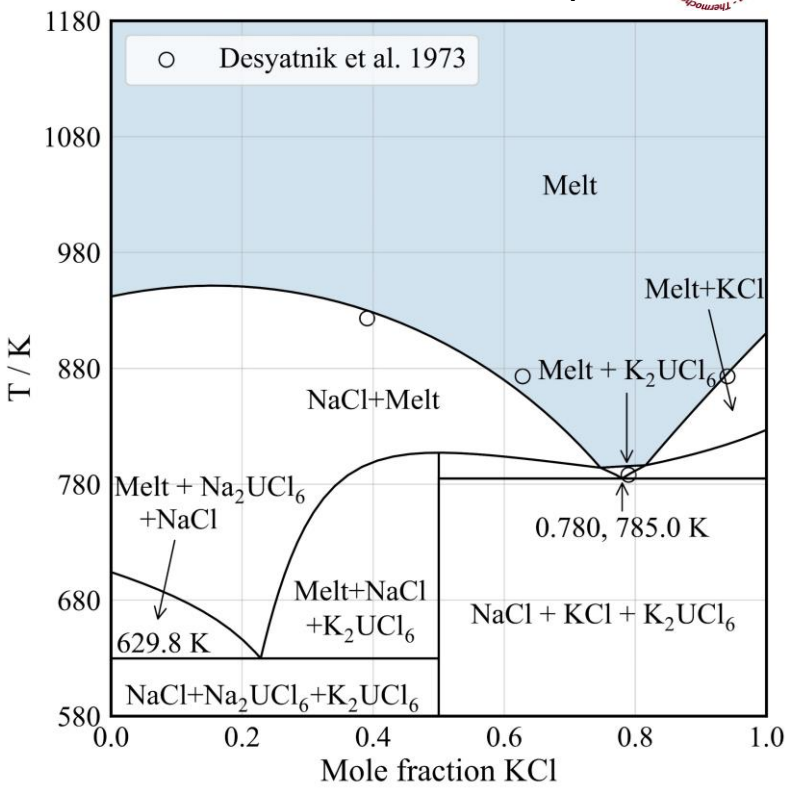
Examples: Computed NaCl-KCl-$CrCl_2$ and NaCl-KCl-UCl_4 Systems

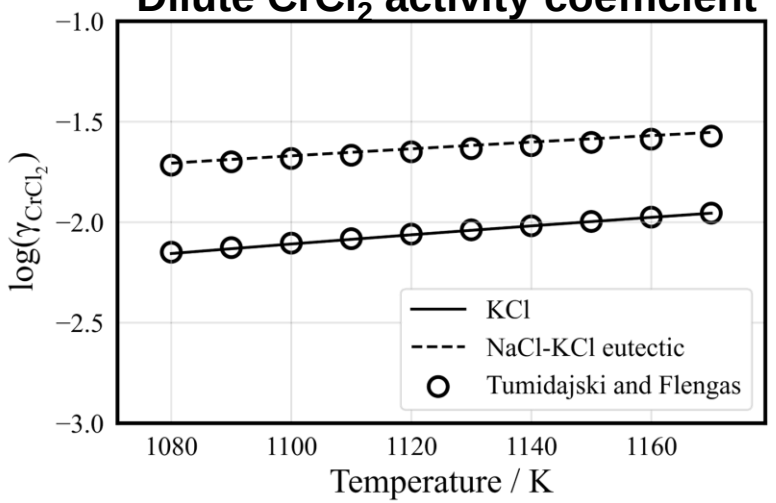
K_2CrCl_4-NaCl



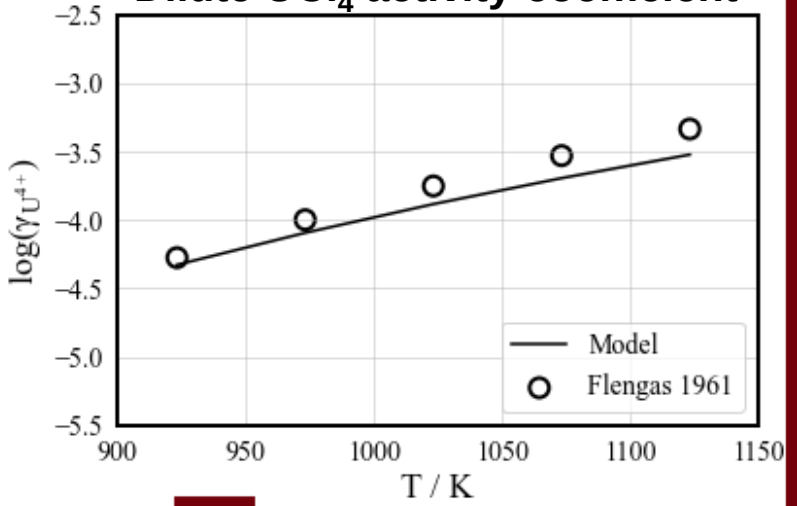
NaCl-KCl Section 20mol% UCl_4



Dilute $CrCl_2$ activity coefficient



Dilute UCl_4 activity coefficient



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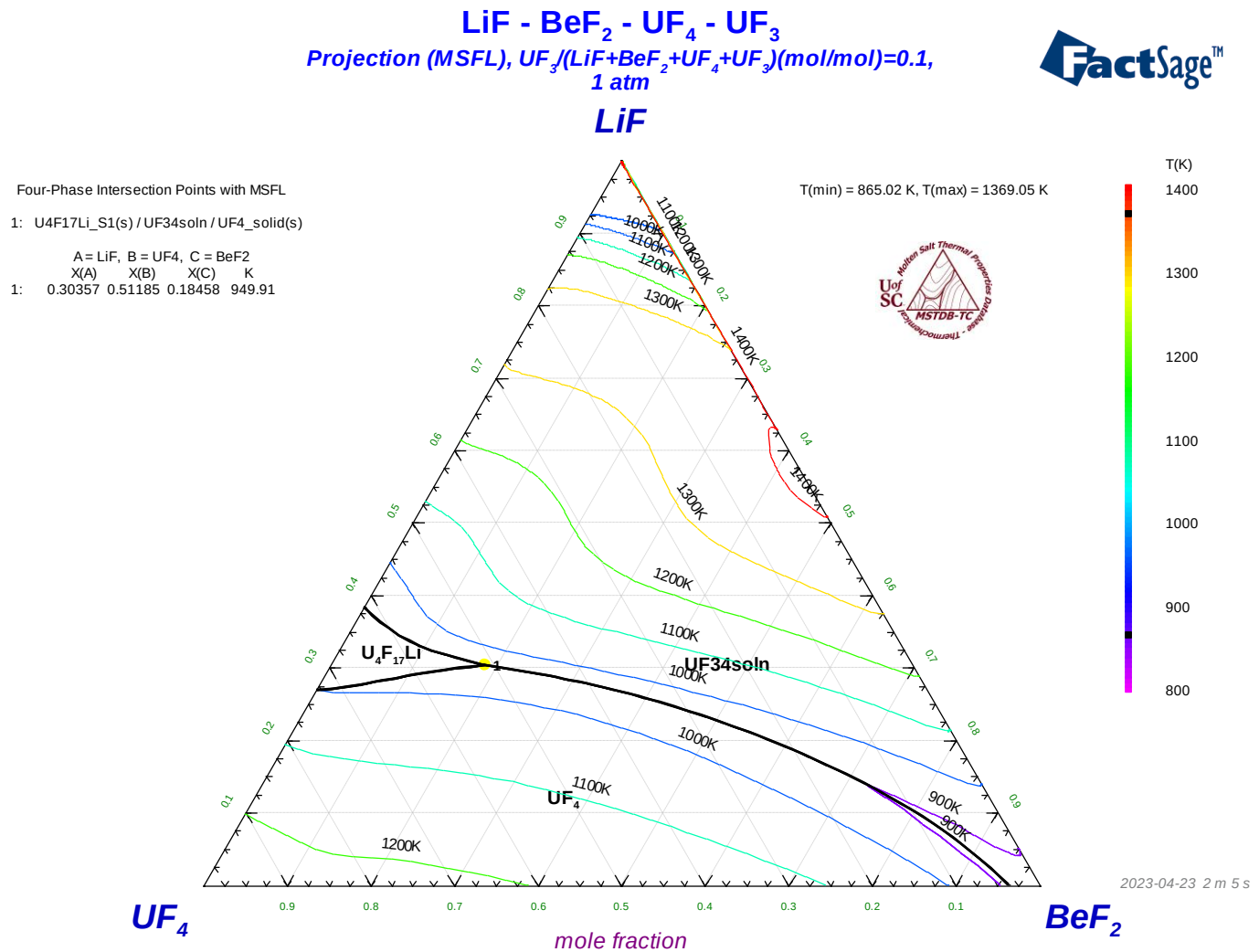
Example: Liquidus Projections for Complex Phase Equilibria

- Isopleths as pseudo-ternary diagrams are easily computed
- Example is the LiF-BeF_2-UF_4 liquidus projection where all compositions contain 0.1 mol fraction UF_3
- Eutectic point and univariant lines are displayed, with first-precipitating phases identified



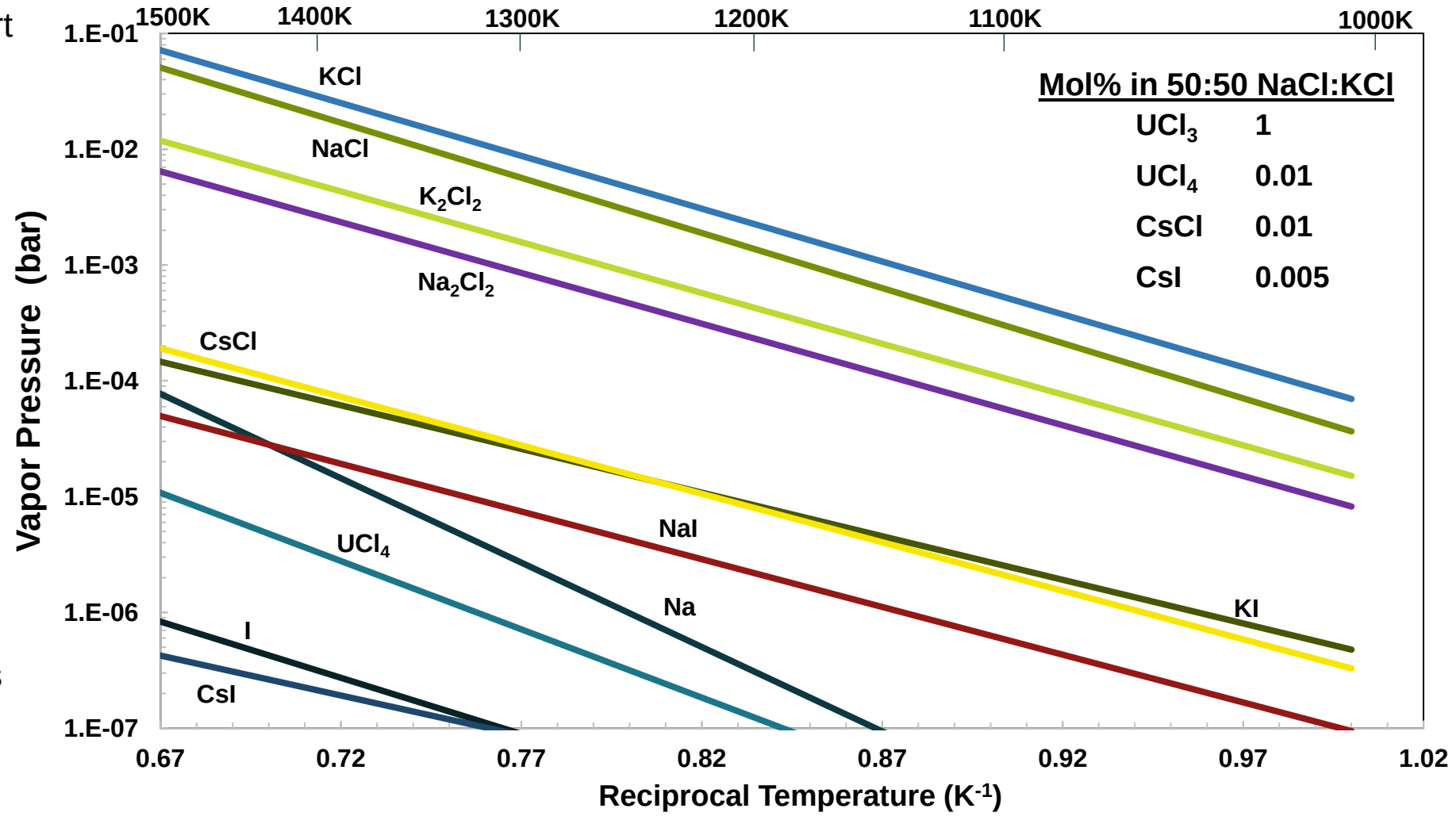
Applications: Computing Vapor Pressures Over Salt Melt

Required for predicting transport
- Gas spaces
- Within noble gas bubbles

Necessary for source terms for accident analysis
- Cesium and iodine species of most concern

Calculation realistic in that
- Chlorine potential fixed by UCl_3:UCl_4 ratio
- Cesium > iodine content

Example observations
- Alkali chlorides have appreciable vapor pressures
- CsCl and KI dominant cesium and iodine species



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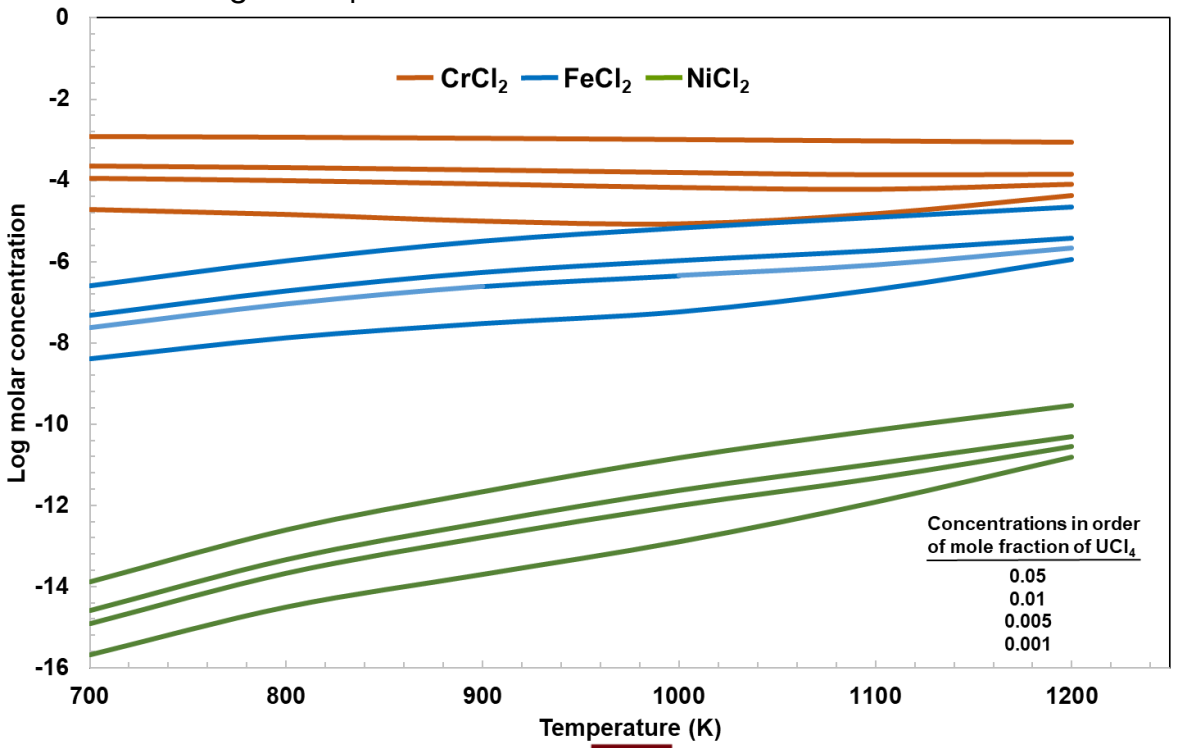
Applications: Computing Equilibria for Modeling Corrosion

Using equilibrium calculations to assess corrosion requires applying appropriate constraints

- Simple computing of the solubility of a corrosion product halide in salt melt is not of value (it will be large)
- Computing alloy-salt equilibria is required to get the limit of corrosion product concentration in melt
- Computing individual metal equilibria can be reasonably accurate, however use of alloy models and thus accurate component activities in the alloy is best (separate alloy database required, e.g., SGTE*)
- Results meaningful only if halide potential is fixed, e.g., ratio UCl_3:UCl_4

Eutectic KCl-$MgCl_2$-5 mol% UCl_3 with 316SS

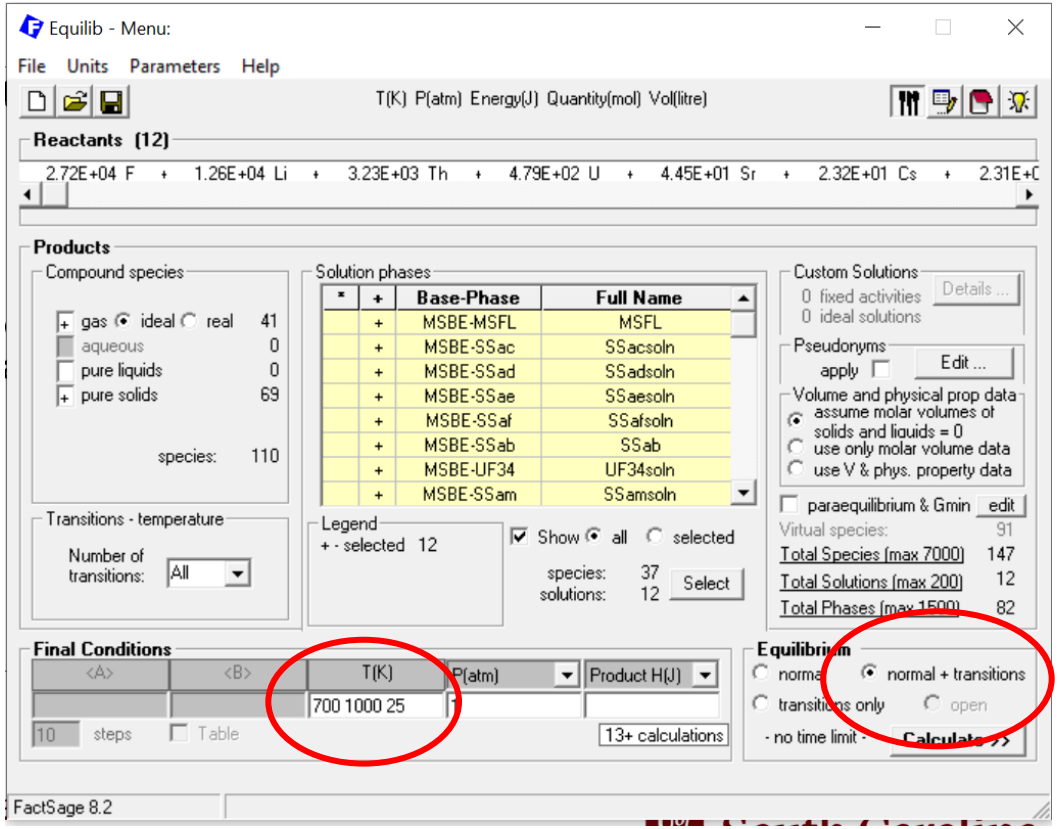
- **Databases**
  - MSTDB-TC Ver. 1.3
  - SGTE
- **Computed Cr, Fe, Ni concentrations**
  - Higher UCl_4/content relative to UCl_3 increases MCl_2 concentrations and thus corrosion rate
  - $CrCl_2$ dominant, but $FeCl_2$ can be significant
  - Surprisingly constant $CrCl_2$ with temperature (also seen experimental in fluoride systems)

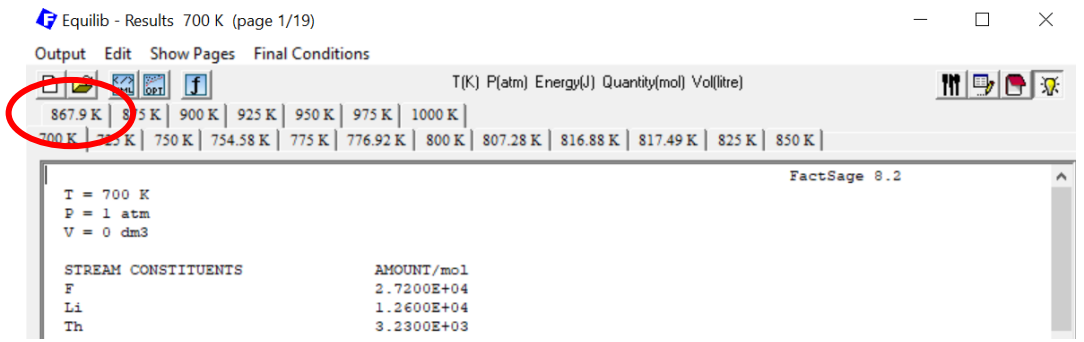


Example: Molten Salt Fast Reactor Salt Behavior Under Burnup

- MSFR Serpent depletion calculations for fresh fuel composition (mol fraction)
  - LiF: 0.7750
  - ThF_4: 0.1988
  - UF_4: 0.0263
- At 80 GWd/t burnup (surrogate elements used in absence of data in MSTDB-TC)

Element	Atom Fraction
F	62.26528
Li	28.80787
Th	7.40335
U	1.12814
Sr	0.12658
Ba	0.06685
Cs	0.06590
Rb	0.05771
Nd	0.00010
Ce	0.00005
La	0.00004
Pu	0.00002





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Precipitation Conditions For Fission Products at 80 GWd/t

- Transitions option finds the points at which phase assemblages change
- For fresh fuel, the first transition from the melt is at 790.5K where LiF precipitates
- For the burnup composition, the first transition from the melt is at 867.9K where the (Li,Rb,Cs)F solid solution phase precipitates
- Burnup has therefore raised the temperature for the first precipitation of a salt phase by 87K

*T = 867.90 K
P = 1 atm
V = 0 dm3

STREAM CONSTITUENTS	AMOUNT/mol
F	2.7200E+04
Li	1.2600E+04
Th	3.2300E+03
U	4.7900E+02
Sr	4.4500E+01
Cs	2.3200E+01
Ba	2.3100E+01
Rb	2.0200E+01
Ce	2.1800E-02
La	1.7700E-02
Nd	4.5700E-02
Pu	3.3500E-03

PHASE: gas_ideal	EQUIL AMOUNT mol	MOLE FRACTION	FUGACITY atm
Rb	0.0000E+00	4.0625E-01	7.9936E-09
FLi	0.0000E+00	2.7677E-01	5.4459E-09
Li2F2	0.0000E+00	1.4403E-01	2.8341E-09

PHASE: MSFL	mol	MOLE FRACTION	ACTIVITY
LiF	1.2600E+04	7.6736E-01	4.3749E-01
U2F8	7.1814E-02	4.3736E-06	3.6222E-08
[illegible]F4	3.2300E+03	1.9671E-01	2.5343E-02
UF3	4.1487E+02	2.5266E-02	1.2628E-01
PuF3	3.3500E-03	2.0402E-07	1.0438E-07
RbF	2.0200E+01	1.2302E-03	5.7619E-04
LaF3	1.7700E-02	1.0780E-06	1.5927E-06
CsF	2.3200E+01	1.4129E-03	5.3665E-06
CeF3	2.1800E-02	1.3276E-06	3.9050E-07
NdF3	4.5700E-02	2.7832E-06	4.3451E-06
U[VII]F	6.3991E+01	3.8971E-03	1.8245E-10
SrF	4.4500E+01	2.7101E-03	7.5442E-03
BaF	2.3100E+01	1.4068E-03	3.9162E-03
U[VI]F	1.5109E-06	9.2014E-11	1.8245E-10
TOTAL:	1.6420E+04	1.0000E+00	1.0000E+00

System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Pu	3.3500E-03	0.81740	7.6799E-08	5.5244E-07
U	479.00	1.1402E+05	1.0981E-02	7.7058E-02
Th	3230.0	7.4948E+05	7.4048E-02	0.50654
Nd	4.5700E-02	6.5919	1.0477E-06	4.4551E-06
Ce	2.1800E-02	3.0545	4.9977E-07	2.0644E-06
La	1.7700E-02	2.4586	4.0578E-07	1.6617E-06
Ba	23.100	3172.3	5.2957E-04	2.1440E-03
Cs	23.200	3083.4	5.3187E-04	2.0839E-03
Sr	44.500	3899.1	1.0202E-03	2.6352E-03
Rb	20.200	1726.4	4.6309E-04	1.1668E-03
F	27200.	5.1676E+05	0.62357	0.34925
Li	12600.	87457.	0.28886	5.9108E-02

PHASE: SSamsoln	mol	MOLE FRACTION	ACTIVITY
LiF	0.0000E+00	1.0000E+00	1.0000E+00
[illegible]F	0.0000E+00	3.4249E-08	1.1179E-03
CsF	0.0000E+00	7.3144E-09	2.4706E-04
TOTAL:	0.0000E+00	1.0000E+00	1.0000E+00

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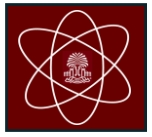
Questions in the Chat or by Email After the Workshop

Acknowledgements:
U.S. Department of Energy Office of Nuclear Energy, under the Nuclear Energy Advanced Modeling and Simulation Program and the Molten Salt Reactor Program under subcontract CW21750 administered by the Oak Ridge National Laboratory, operated by UT-Battelle, L.L.C., for the U.S. Department of Energy under contract DE-ACO5-000R2275



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South Carolina

OntarioTech Engineering & Applied Science

Use of MSTDB-TC with Thermochimica and Case Studies

M.H.A. Piro, M. Poschmann*

Molten Salt Thermal Properties Database Workshop (Virtual)

April 25, 2023

* Currently at Canadian Nuclear Laboratories

Outline

- What is Thermochimica and how does it work?
- What can you do with Thermochimica + MSTDB-TC?
- How do you know it’s right (QA)?
- Related peripheral activities

What is Thermochimica?

e.g., MSTDB-TC

- Open-source thermodynamics software.
  - **Input:** Temperature, pressure, composition, database.
  - **Output:** Phases, phase speciation, thermodynamic properties.

- Software:
  - Written mainly in F90 with Python and C++ wrappers.
  - Requires LAPACK libraries.
  - Maintained on github.
  - Supports almost all major classes of models.

https://nuclear.ontariotechu.ca/piro/thermochimica/

How does Thermochimica Work?

Gibbs energy equations are empirically derived.

- The integral Gibbs energy of a system is:

$$G = \sum_{\lambda=1}^{\Lambda} n_\lambda g_\lambda + \sum_{\omega=1}^{\Omega} n_\omega g_\omega$$

- Taylor series expansion yields:

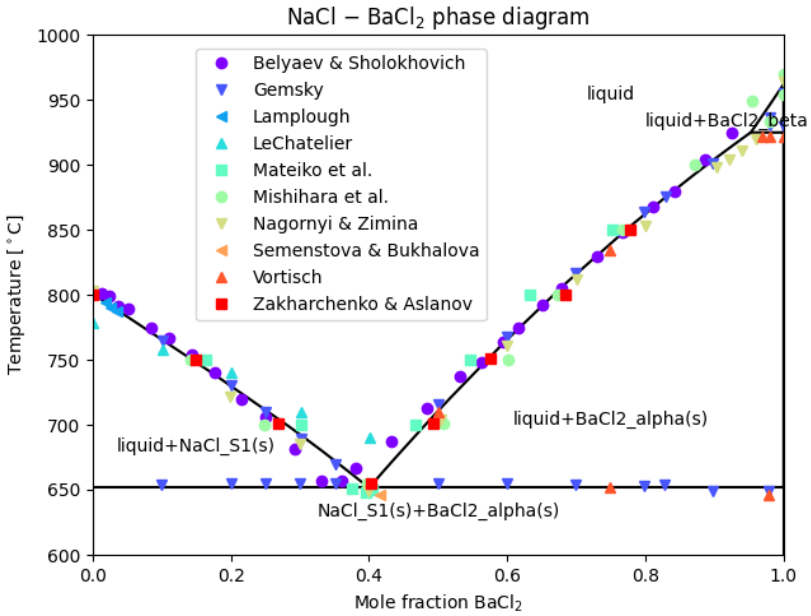
$$L = G - \mathbf{\Gamma}\phi \qquad \phi_j = \sum_{\lambda}\sum_{i} n_{i(\lambda)}\nu_{i,j} + \sum_{\omega} n_\omega \nu_{\omega,j} - b_j$$

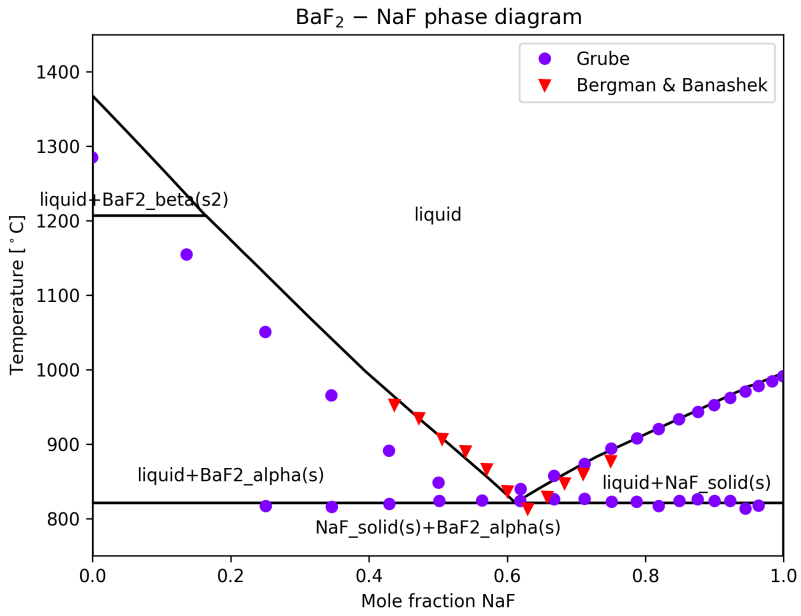
$$\nabla^2 L\delta = -\nabla L$$

Yes, experimental validation data.

Case Study #1: Phase Diagram Generation

A GUI was recently created, which can generate phase diagrams (among other things).
These models were developed by Ontario Tech for the MSTDB-TC.



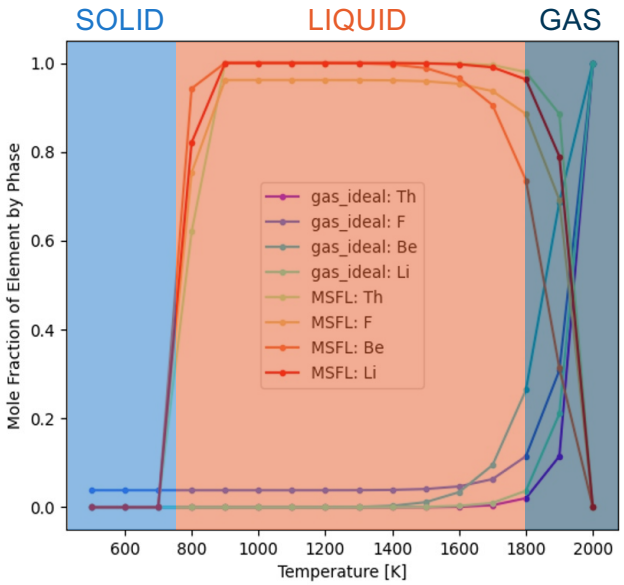


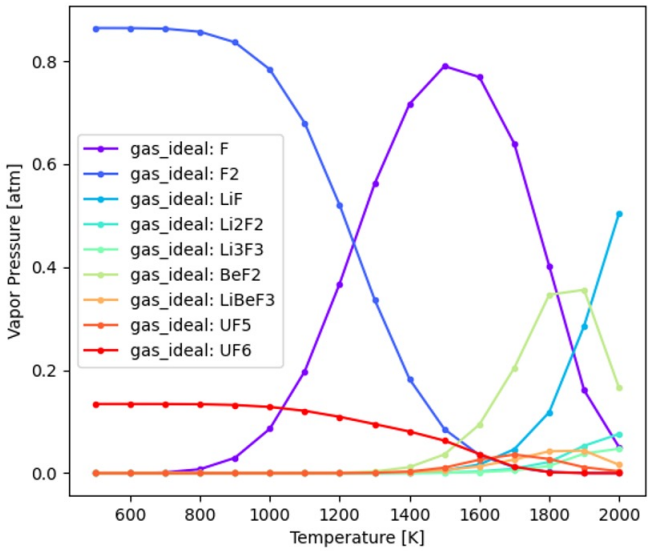
M. Poschmann, M.H.A. Piro, “Thermodynamic Assessments of the Pseudo-Binary {Ba,Sr}-{Na,K} Fluoride and Chloride Salt Systems”, Ontario Tech, Oshawa, Canada (2022).

No experimental validation data.

Case Study #2: Salt/Gas Speciation

H. Patenaude (UNLV) performed analyses of irradiated salt (FLiBe + fuel + FPs) using MSTDB-TC and predicted phase equilibria and gas partial pressures.





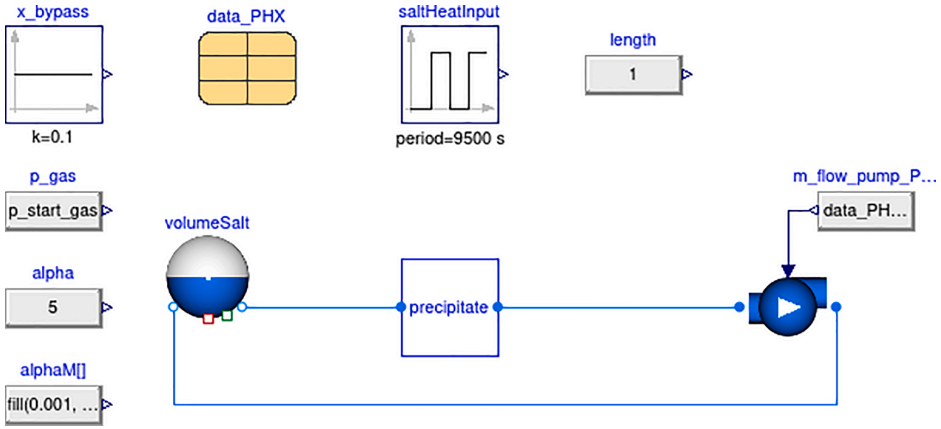
Disclaimer: These simulations should be viewed as demonstrations of capability development.

H.K. Patenaude, “Thermodynamic predictions of irradiated molten fluoride salts”, UNLV, Las Vegas, USA (2022).

No experimental validation data.

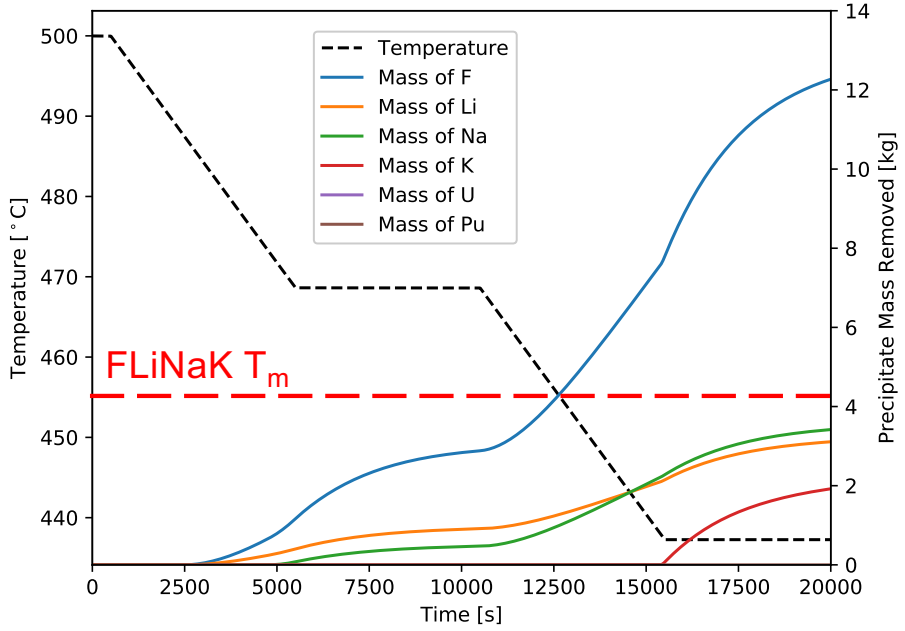
Case Study #3: Precipitate Filtration

TRANSFORM system code



Disclaimer: These simulations should be viewed as demonstrations of capability development.

Precipitate Filtration Removal

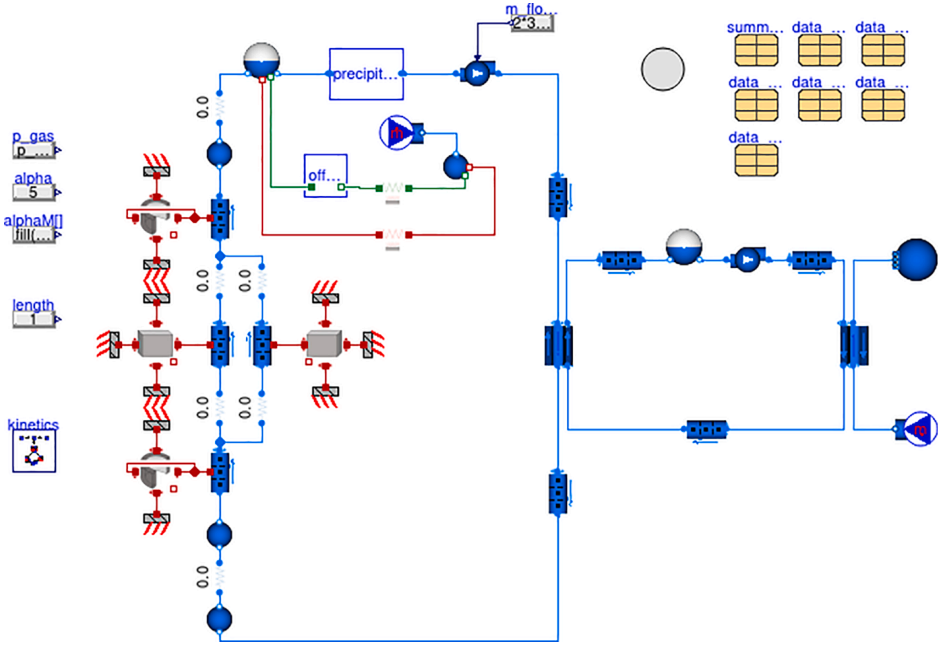


M. Poschmann, M.H.A. Piro, M.S. Greenwood, Nucl. Eng. Des., 390 (2022) 111695.

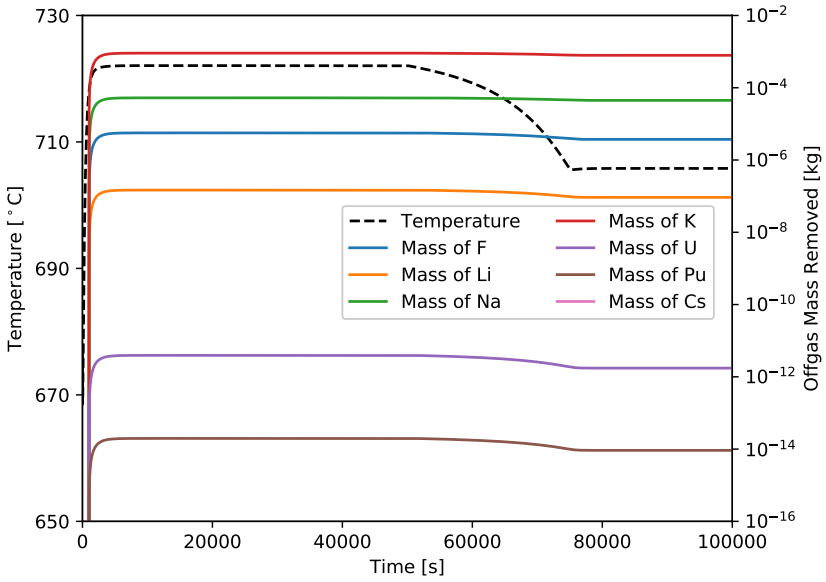
No experimental validation data.

Case Study #4: Loss of Flow Accident

TRANSFORM system code



Off-gassing Removal



Disclaimer: These simulations should be viewed as demonstrations of capability development.

M. Poschmann, M.H.A. Piro, M.S. Greenwood, Nucl. Eng. Des., 390 (2022) 111695.

No experimental validation data.

Case Study #5: Severe Accident Analyses

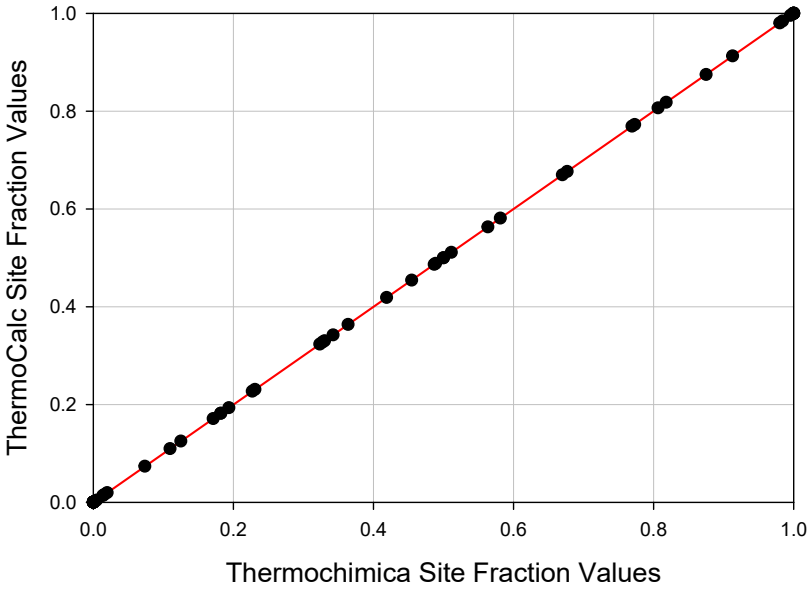
- A previous project in partnership with Sandia National Labs coupled MELCOR with Thermochimica, including MSR applications.
  - Predict fission product speciation, which can feed into source term calculations.

- Simulations of severe accident behaviour has high value to industry and regulator for safety and licensing applications.

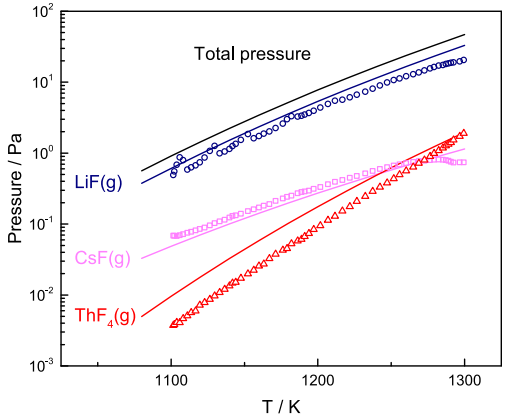
F. Gelbard, B.A. Beeny, L.L. Humphries, K.C. Wagner, M. Poschmann, M.H.A. Piro, Nucl. Sci. Eng., in-press.

Quality Assurance: Benchmarking

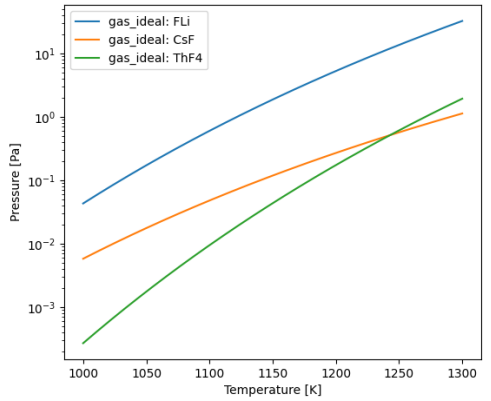
LWR Corium Benchmark (TAF-ID)



Vapour Pressure Benchmark with Experiments



Computed with FactSage

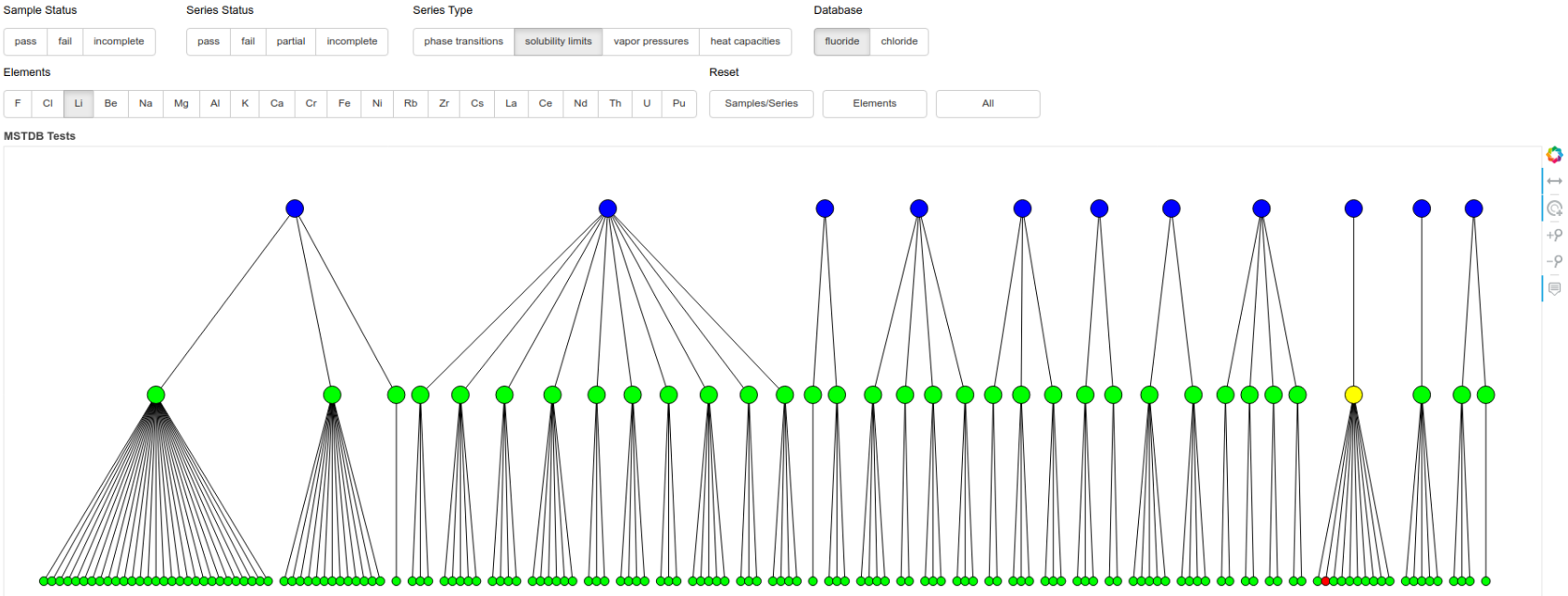


Computed with Thermochimica

B. Breeden, MASc Thesis, Ontario Tech University, Oshawa, ON (2021).

Quality Assurance: Unit Test Validation

- 1168 tests from 88 experimental sources have been compiled.
- See Max Poschmann's presentation for more details.

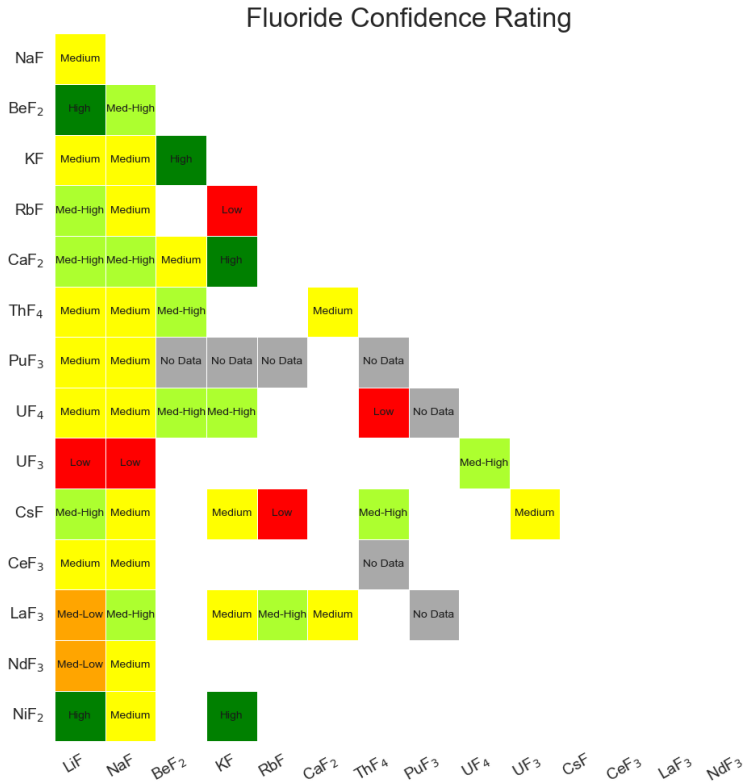


Quality Assurance: Integral Test Validation

- Integral tests to validate codes and models related to MSR behaviour are sparse.

Peripheral Activities: Computational

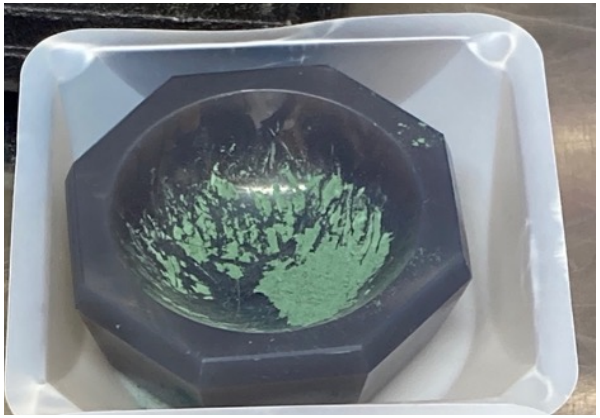
- Another PhD student (N. Scuro) is working on OpenFOAM + Thermochimica coupling for MSR applications.
- Knowledge gap identification in databases, driven by stakeholder needs.
  - Discussed by M. Poschmann earlier.

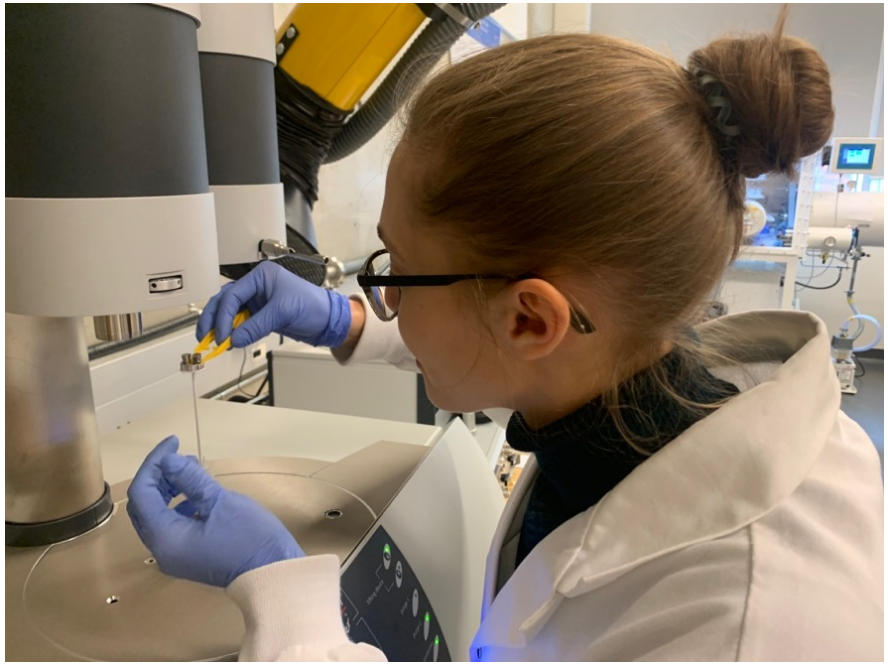


M. Piro, P. Bajpai, M. Poschmann, Idaho National Laboratory, INL/RPT-22-69782, Idaho, US (2022).

Peripheral Activities: Experimental

- On-going experimental work at Ontario Tech:
  - Focusing on fuel + FPs.
  - Provides validation data for material models.





Conclusions

- Thermochimica + MSTDB-TC are like peanut butter and jam.
  - One can use Thermochimica to generate phase diagrams from the MSTDB-TC, perform calculations related to in-reactor behaviour, or couple with multi-physics codes.
  - Both are freely available.

- Several scenarios being simulated have not been validated.
  - Recommend government agencies to fund more experimental campaigns to validate models/codes (esp. integral experiments).

Acknowledgements

- Thanks to Ted Besmann (UofSC) and Dianne Ezell (ORNL) for putting on this workshop.
- Financial support from Sandia National Laboratories is greatly acknowledged.
- Some of this work was funded by the U.S. Department of Energy's Nuclear Energy Advanced Modeling and Simulation program.
- This research was undertaken, in part, thanks to funding from the Canada Research Chairs program of the Natural Sciences and Engineering Research Council of Canada.

Questions?

https://nuclear.ontariotechu.ca/piro

UF Herbert Wertheim College of Engineering
UNIVERSITY of FLORIDA

TRG
TONKS RESEARCH GROUP

MSTDB-TC applications and use in phase field modeling

Chaitanya Bhave, Michael R. Tonks, Kumar Sridharan, Adrien Couet, Markus Piro, Parikshit Bajpai

POWERING THE NEW ENGINEER TO TRANSFORM THE FUTURE

Acknowledgements

NEAMS
NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

NEUP Nuclear Energy University Program
U.S. Department of Energy

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Idaho National Laboratory

Los Alamos
NATIONAL LABORATORY
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OAK RIDGE
National Laboratory

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Tonks Research Group

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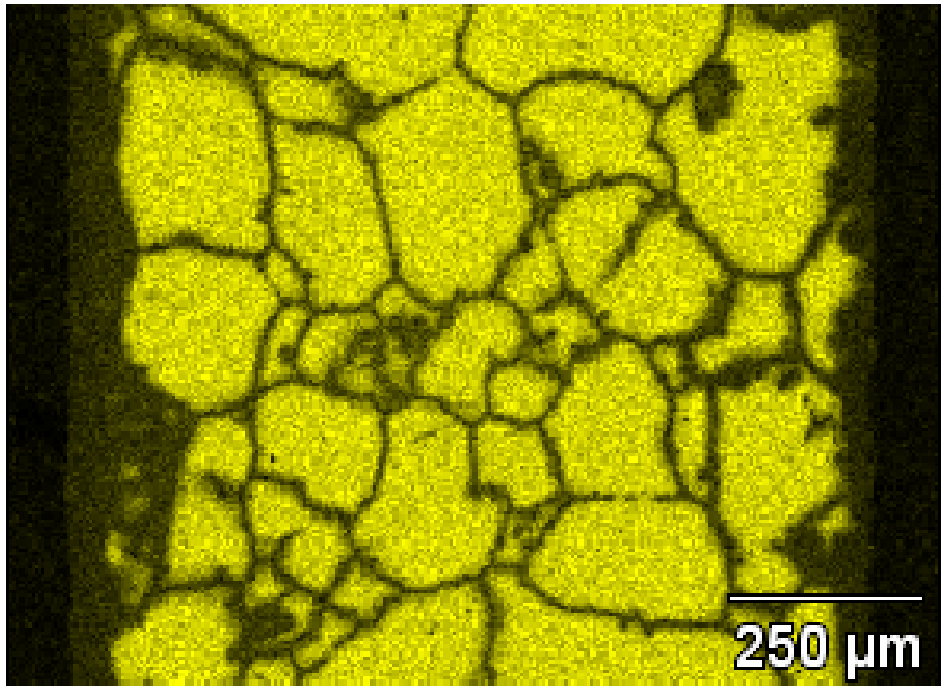
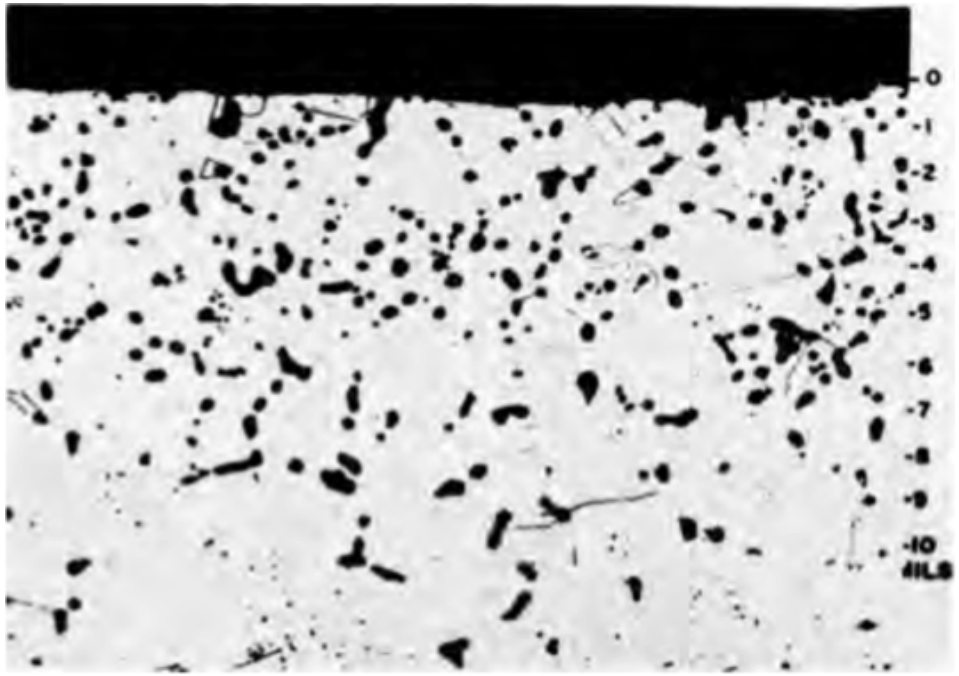
UNIVERSITY

W

Impact of molten salt corrosion on microstructure



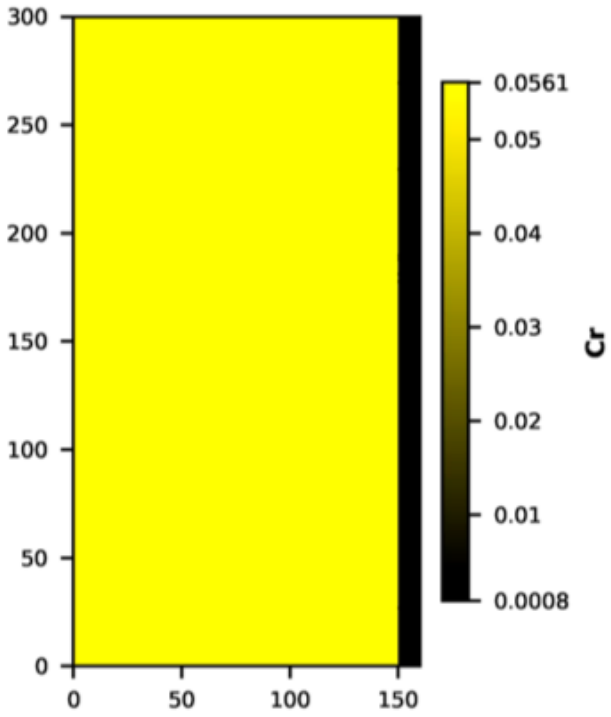
Cr EDS scan of cross section of FLiNaK exposed Incoloy-800H [1]

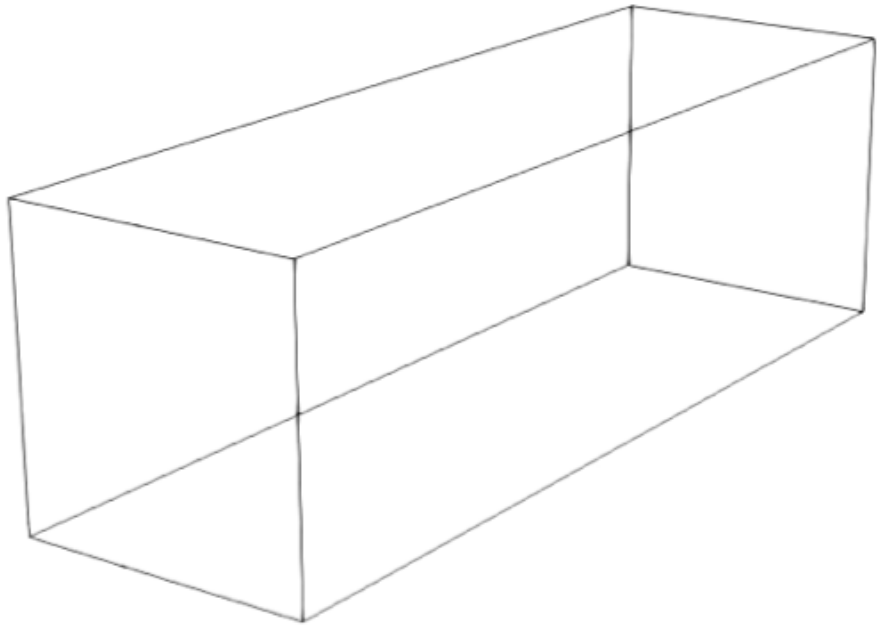


Inconel alloy after exposure to molten fluoride salt high in HF [2]

1. Olson, L. (2009). *Materials Corrosion in Molten LiF-NaF-KF Eutectic Salt*. Ph.D. University of Wisconsin-Madison.
2. Manly, W. et al. (1957). *Aircraft Reactor Experiment - Metallurgical Aspects*. ORNL-2349. [online] Available at: https://www.osti.gov/servlets/purl/4227617 [Accessed 30 Oct. 2019].

We have developed a mesoscale model of alloy corrosion by molten salt using the MOOSE framework





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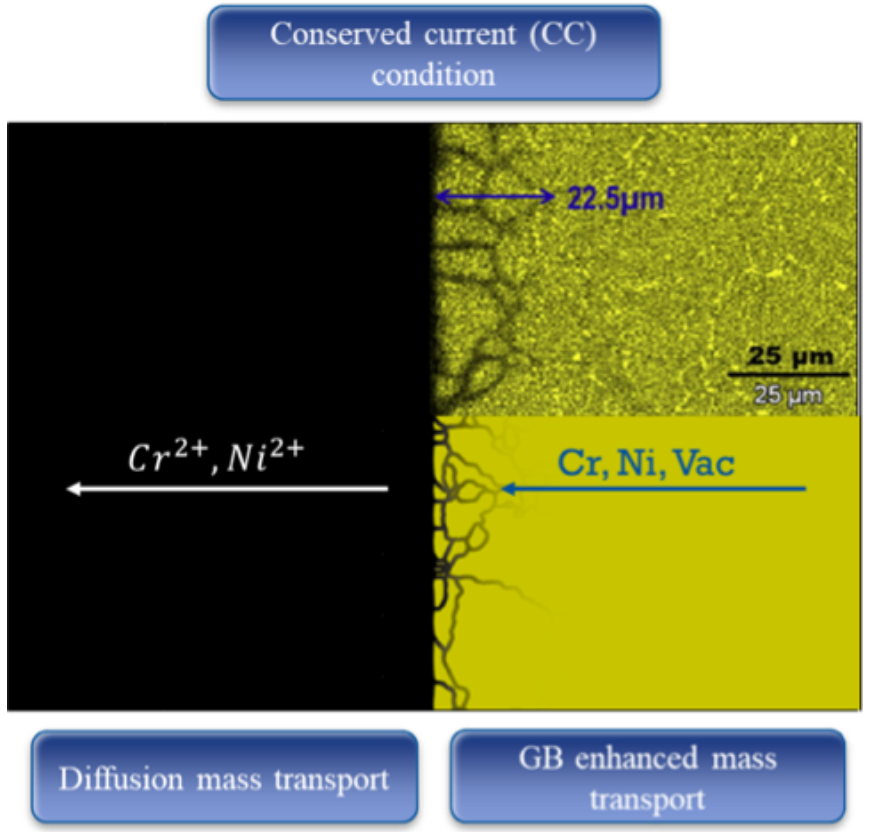
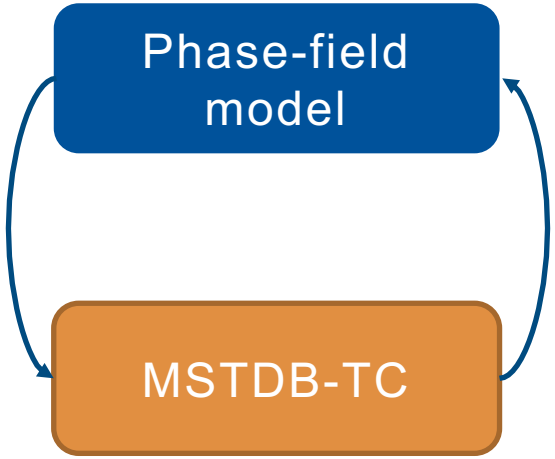
- Phase-field model demonstration



- Using MSTDB-TC with the phase-field model



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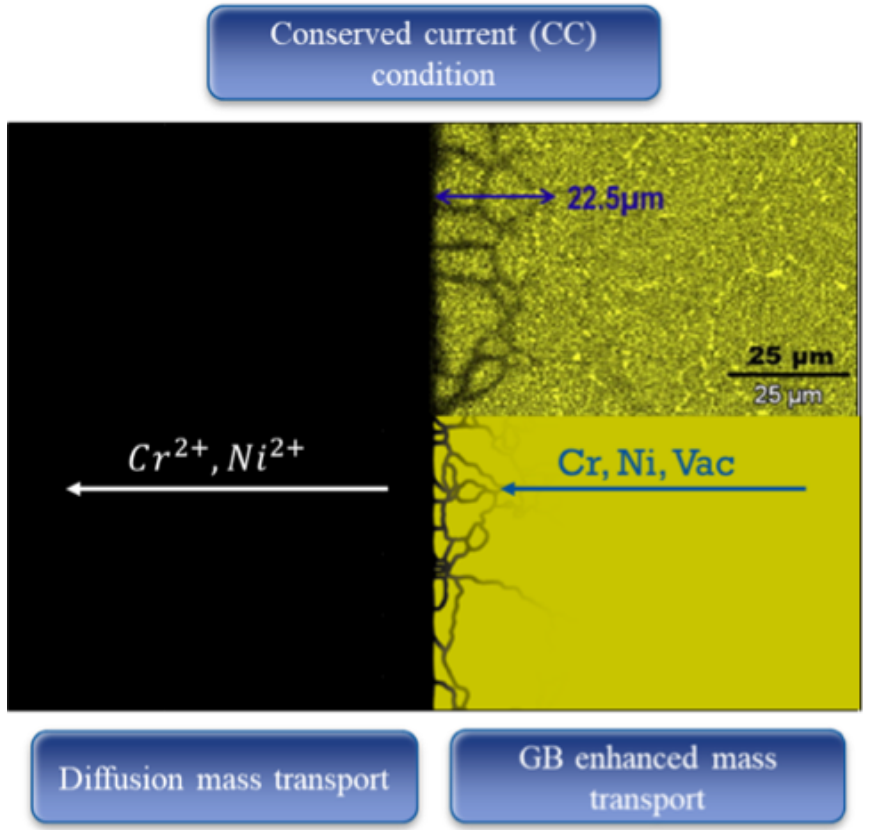

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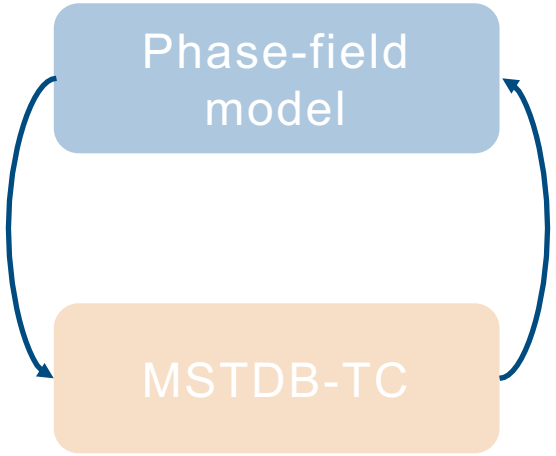

We developed an electrochemical mesoscale model for corrosion of Ni-Cr alloys in molten FLiBe

- Uses the phase field method solved using MOOSE
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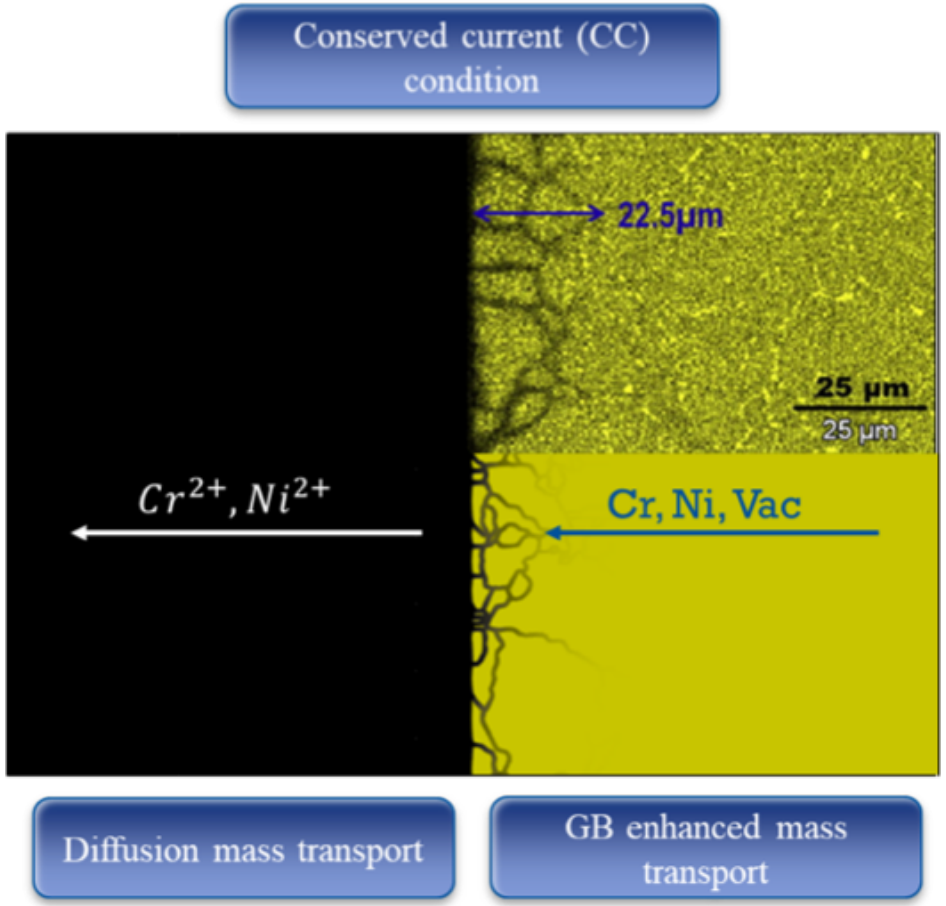
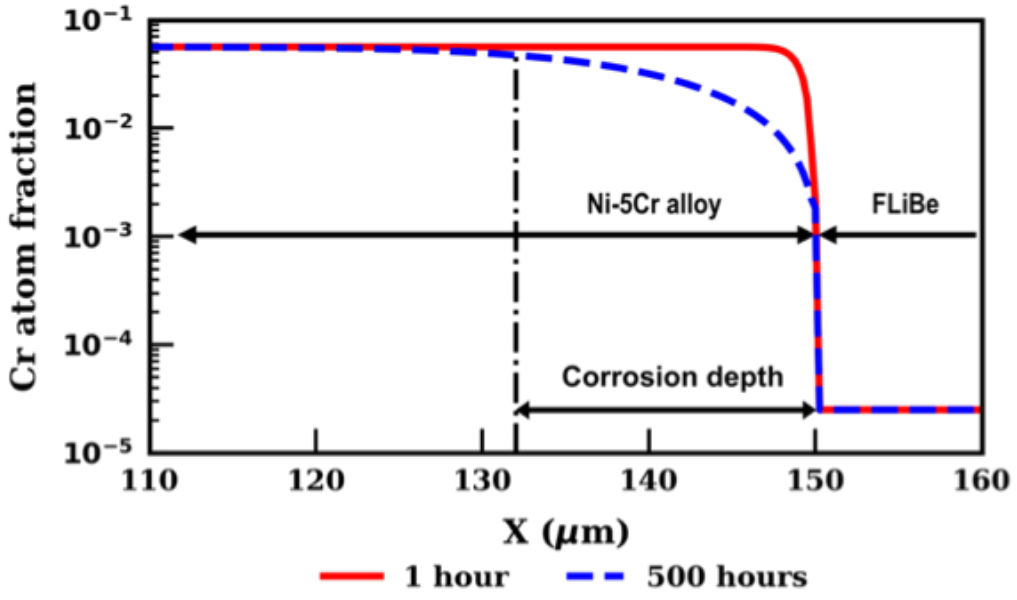
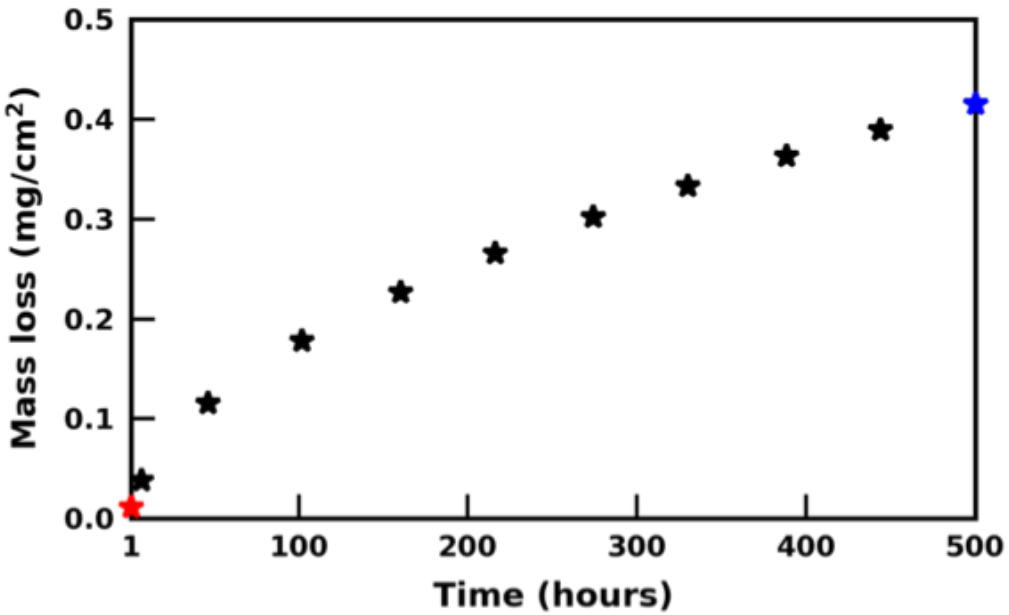
  - Free energy of the alloy
  - Free energy of the salt
  - Interface energy
  - Electric potential
  - Bulk and GB diffusion in alloy
  - Alloy microstructure
- Materials
  - FLiBe
  - Ni-Cr and Fe-Cr alloys



1D simulations make quantitative mass loss predictions

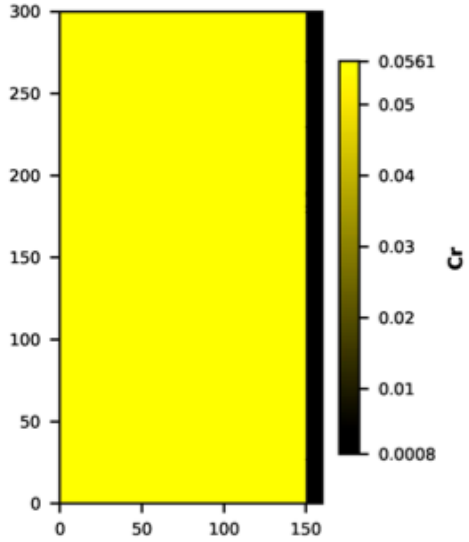


Line scan of Cr atomic fraction in Ni-5Cr



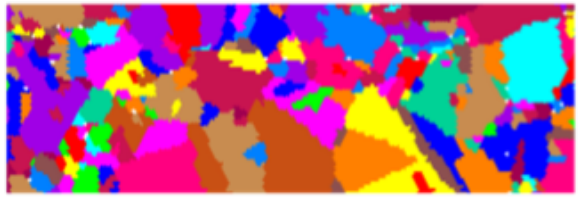
Mass loss in Ni-5Cr during corrosion

2D simulations can capture selective Cr depletion along GBs

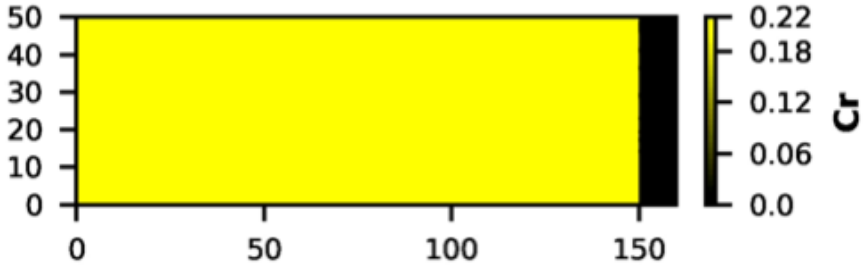


EBSD Simulation

Cr depletion in Ni-5Cr alloy



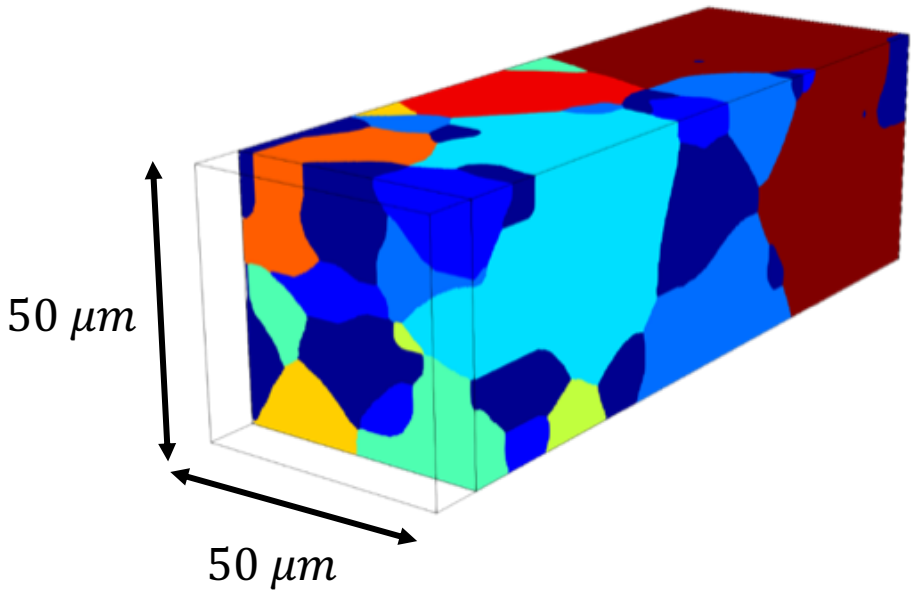
EBSD



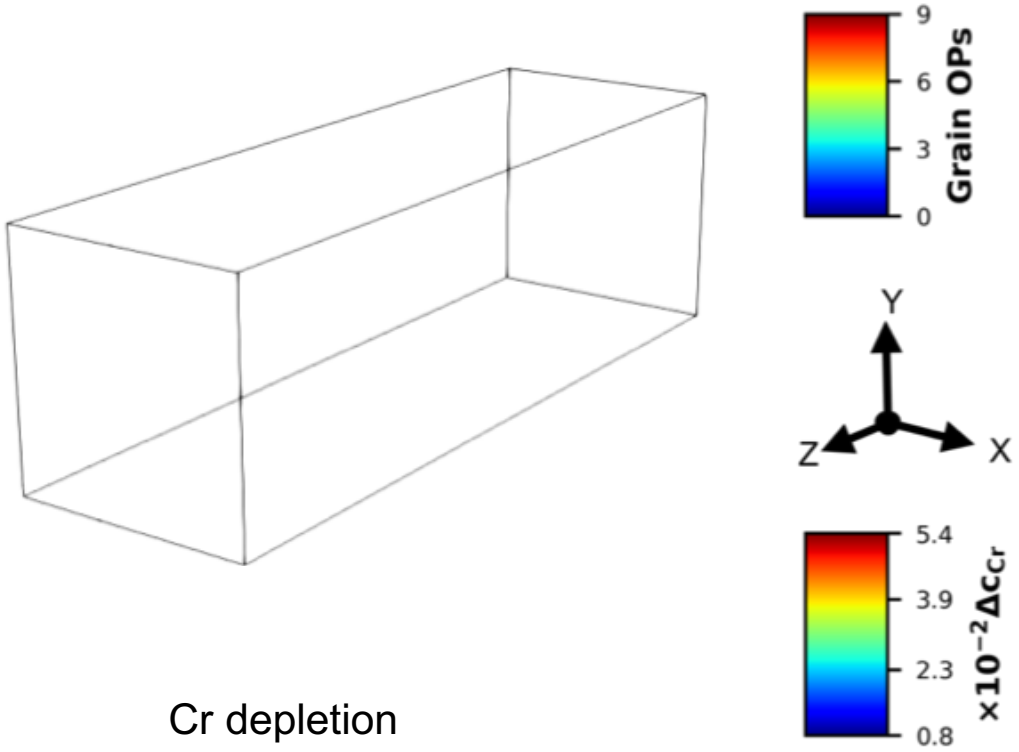
Simulation

Cr depletion in Ni-20Cr alloy

We also simulated Ni-5Cr corrosion in 3D

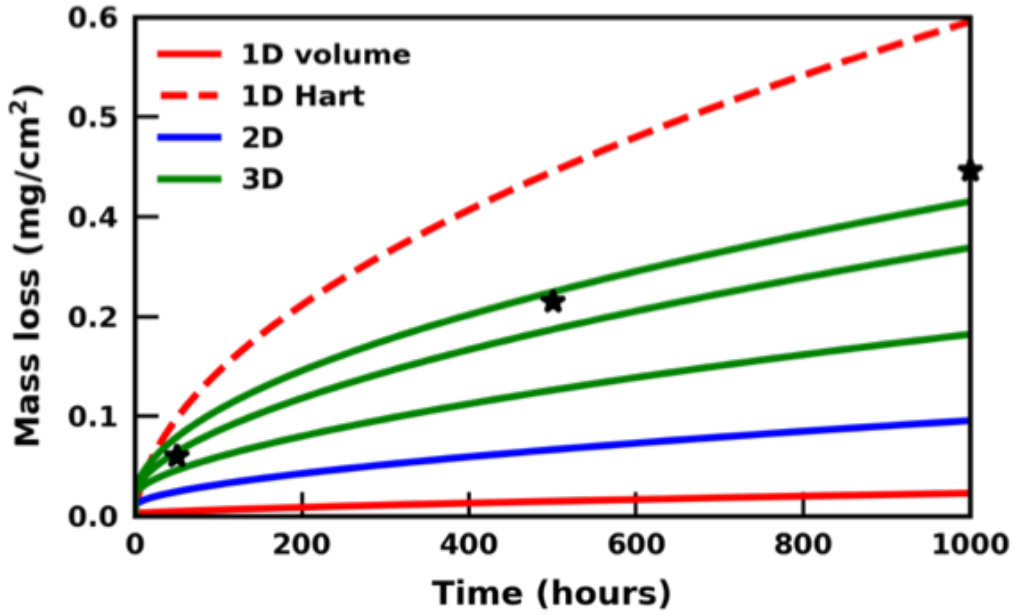


3D microstructure

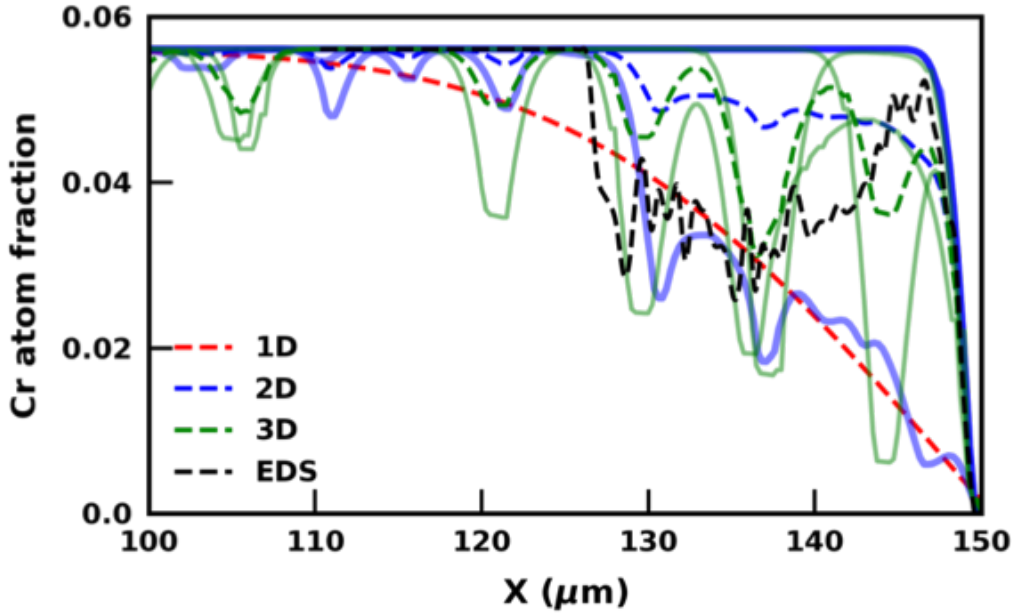


Cr depletion

Validation using Ni-5Cr experimental data

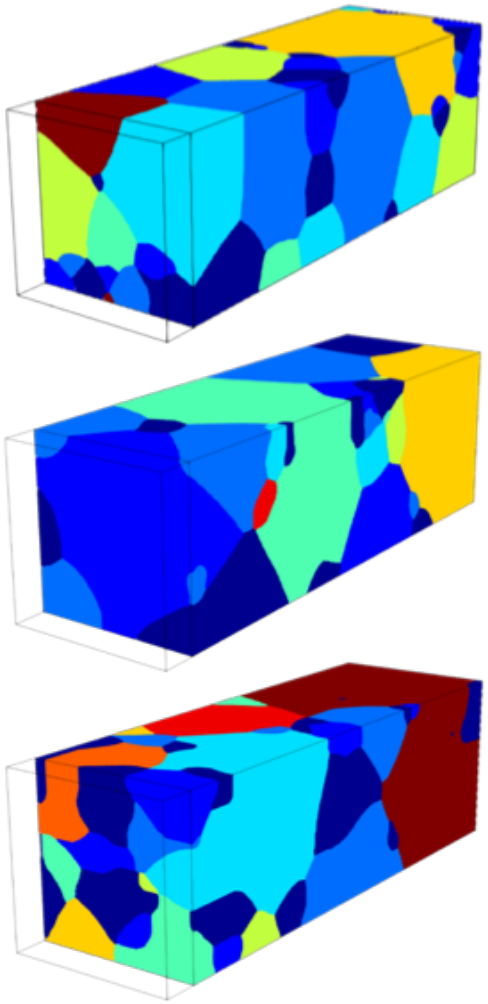


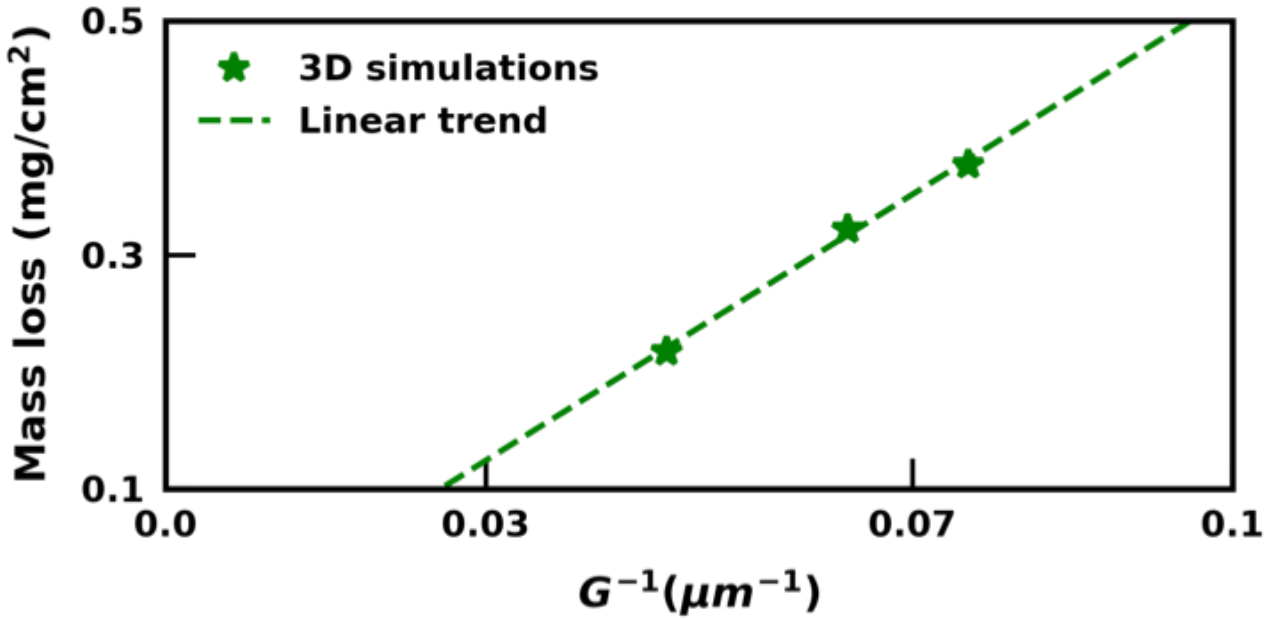
Mass loss comparison



Cr depletion line plot

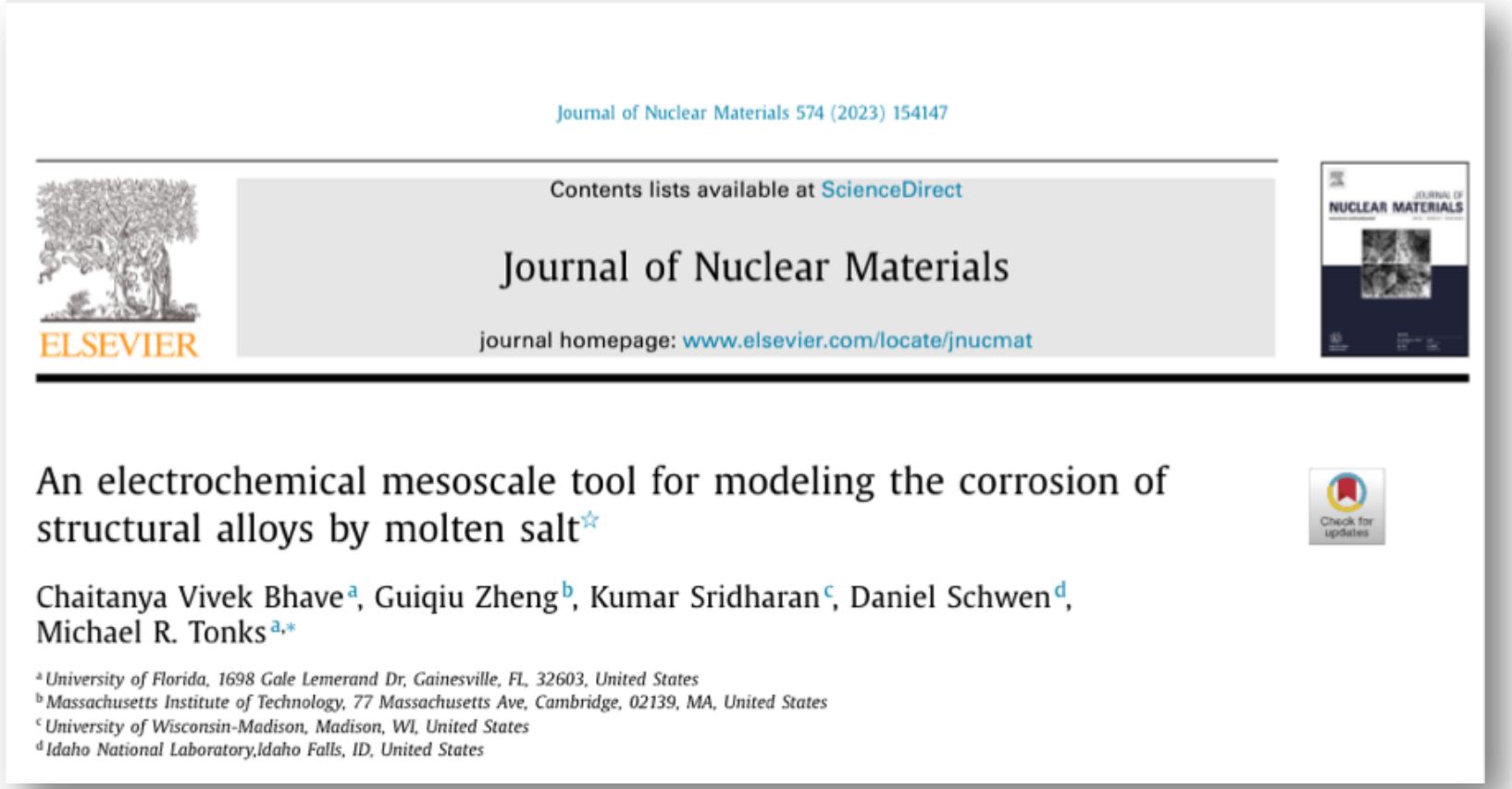
Cr mass loss is proportional to average grain size at surface





Mass loss at 1000 hours vs inverse of projected grain size

See our paper for more information



Journal of Nuclear Materials 574 (2023) 154147

Contents lists available at ScienceDirect

Journal of Nuclear Materials

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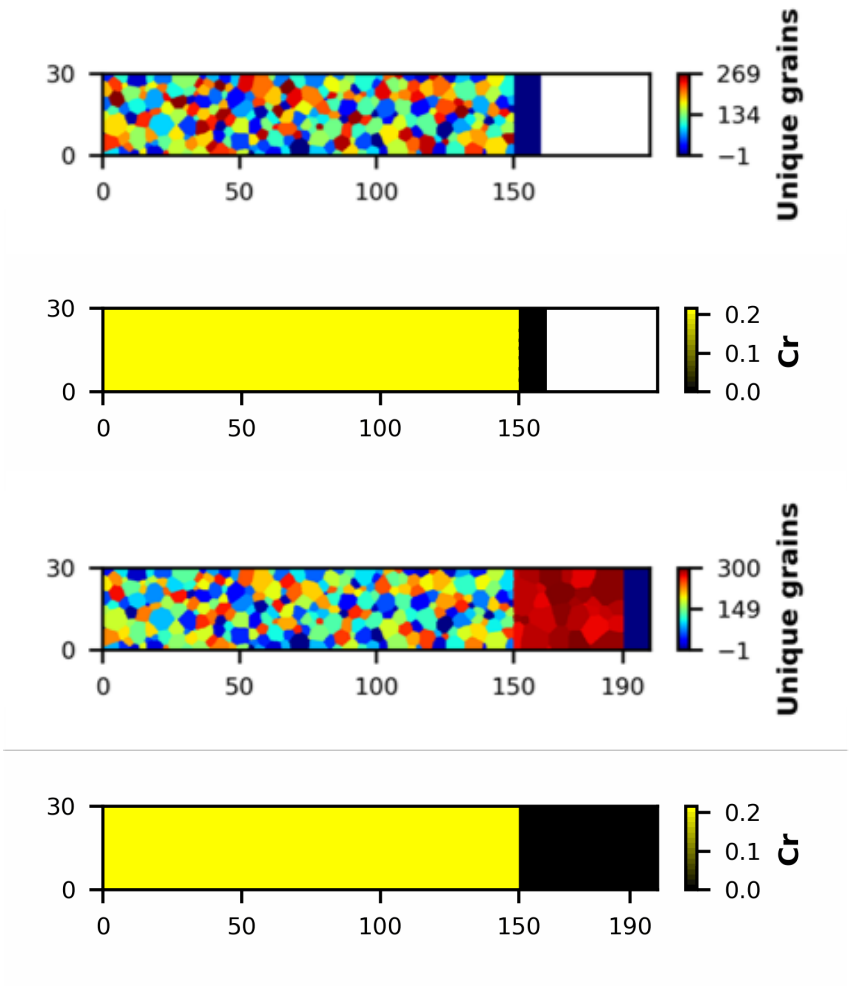
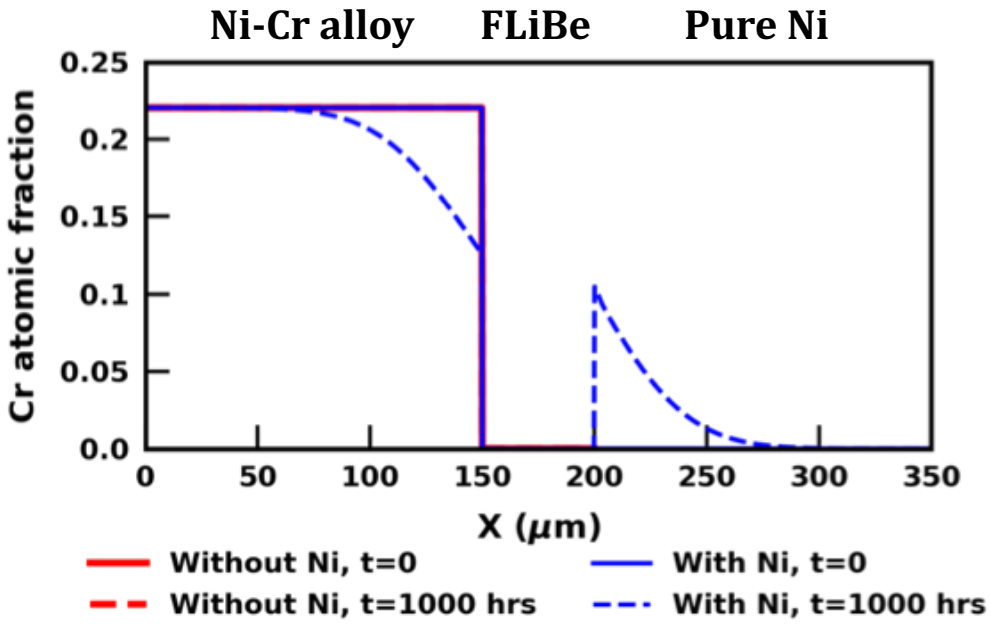
An electrochemical mesoscale tool for modeling the corrosion of structural alloys by molten salt☆

Chaitanya Vivek Bhave[a], Guiqiu Zheng[b], Kumar Sridharan[c], Daniel Schwen[d], Michael R. Tonks[a,*]

[a] University of Florida, 1698 Gale Lemerand Dr, Gainesville, FL, 32603, United States
[b] Massachusetts Institute of Technology, 77 Massachusetts Ave, Cambridge, 02139, MA, United States
[c] University of Wisconsin-Madison, Madison, WI, United States
[d] Idaho National Laboratory,Idaho Falls, ID, United States

We have also applied the model to investigate the impact of coatings and added activity gradient corrosion





Cr atomic profile during activity gradient corrosion

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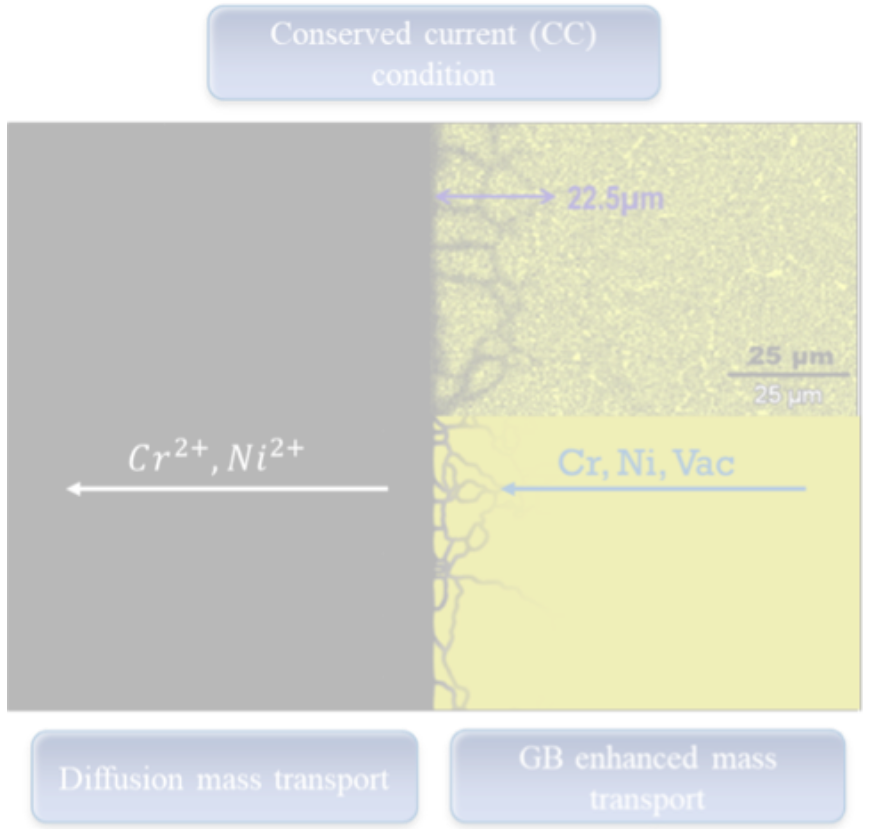
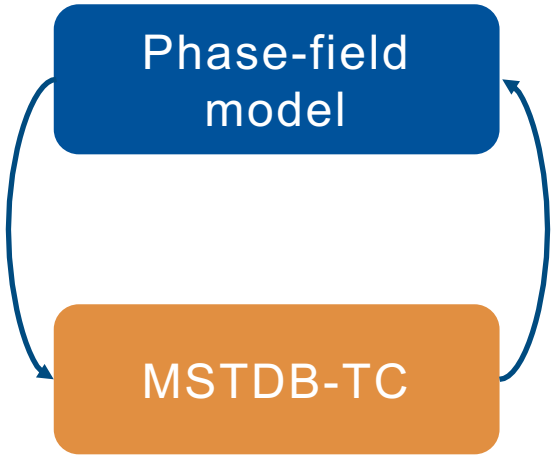
- Phase-field model demonstration



- Using MSTDB-TC with the phase-field model

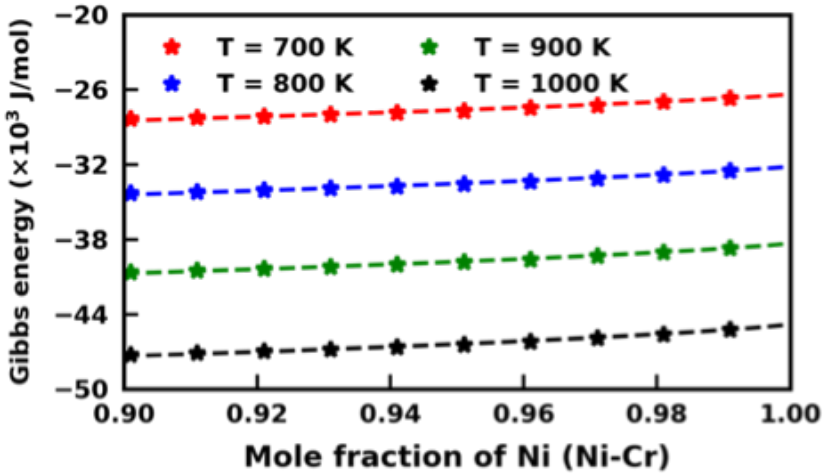


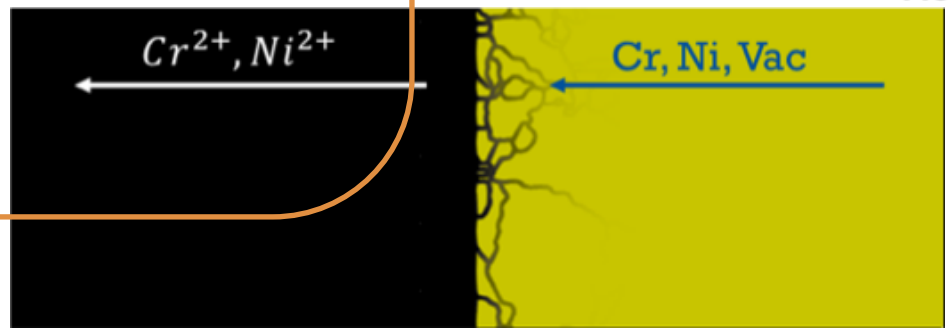
Our model predicts the corrosion by minimizing the overall free energy of the system

- Free energy of the salt
  - $f_s(c_{Cr^{2+}}, c_{Ni^{2+}}, E^0_{Ni/Ni^{2+}}, E^0_{Cr/Cr^{2+}}, E_{F_2/F^-})$
    - $E^0_{Ni/Ni^{2+}}$ and $E^0_{Cr/Cr^{2+}}$ are oxidation potentials
    - E_{F_2/F^-} is the fluoride potential (or Cl potential)
    - Changes with redox potential, which is impacted by impurities in salt
- Chemical potentials
  - $\frac{\partial f_s}{\partial c_{Cr^{2+}}}, \frac{\partial f_s}{\partial c_{Ni^{2+}}}$

From MSTDB-TC!

- Free energy of the alloy





There are various approaches for using the MSTDB-TC with our phase field model, with varying difficulty and computational cost

Manually fit simpler model to MSTDB-TC data

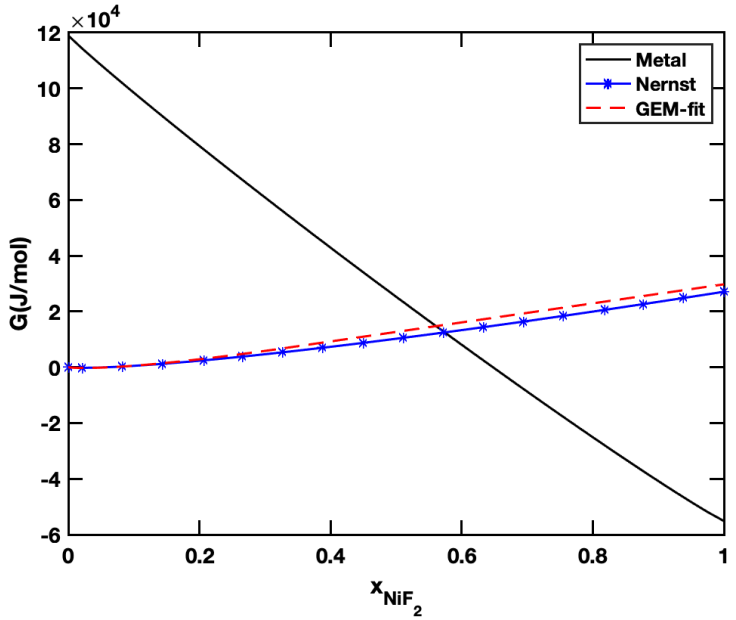
- Computationally efficient
- Time intensive for each system change
- Our current primary approach

Fit model to data from ThermoChimica with MSTDB-TC

- Medium efficiency
- Output new data when the system changes
- Preliminary example complete

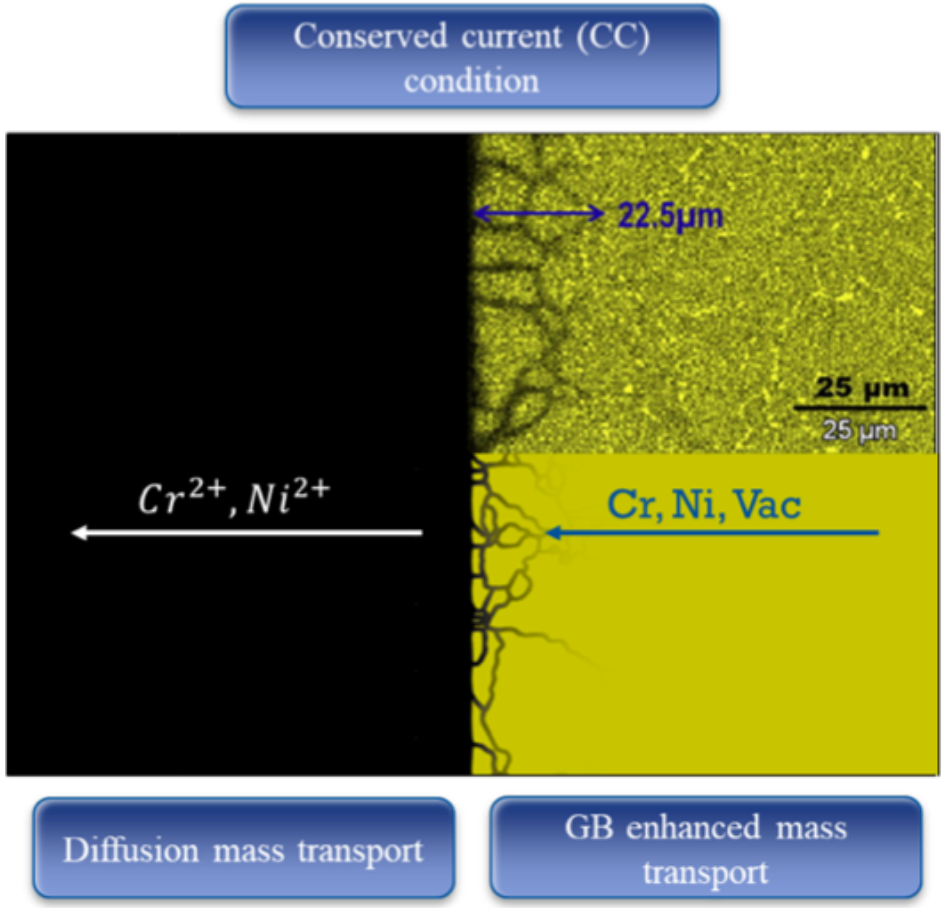
Directly couple MOOSE to ThermoChimica with MSTDB-TC

- Very computationally expensive
- System changes require no additional work



The data available now in the MSTDB-TC and that will be added in the future will enable the expansion of our model

- Additional salts beyond FLiBe
  - FLiNaK (coming soon!)
  - U-bearing salts
  - Chloride salts
- Direct representation of impurities
  - More corrosion products (Fe, Ni)
  - H_2, H_2O, …
  - Fission products



Conclusions

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We developed an electrochemical mesoscale model for corrosion of Ni-Cr alloys in molten FLiBe

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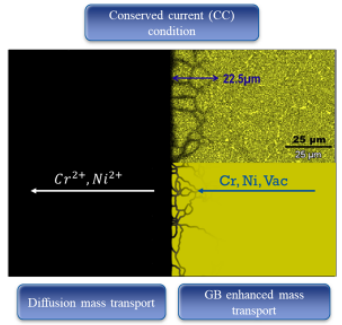

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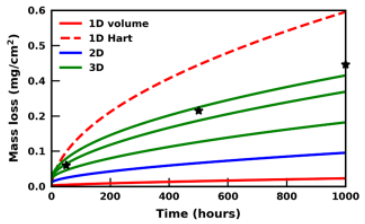

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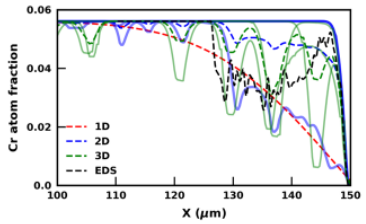

Cr depletion line plot

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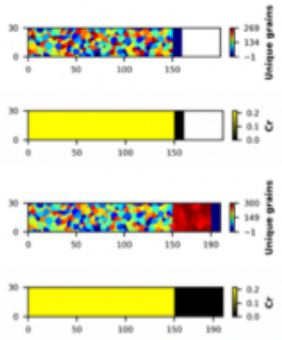

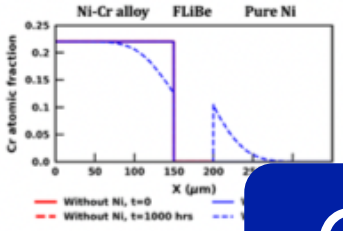

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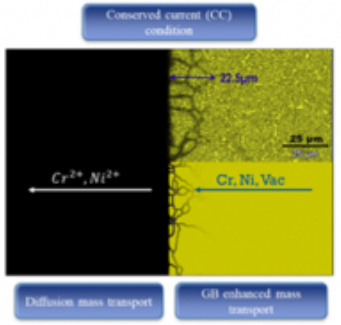


Questions?

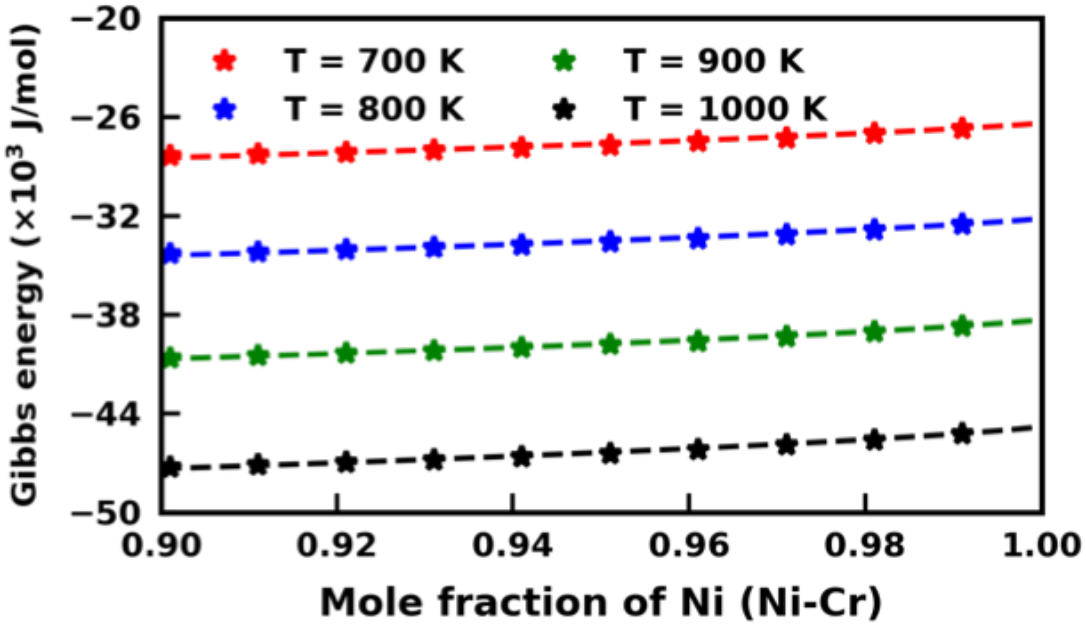
The chemical driving force is defined by alloy and salt free energies taken from CALPHAD databases

- Free energy of Ni, Cr and vacancies in metal phase from ideal solution fit to CALPHAD free energy

$$\Delta_f G^0_{Cr,Ni} = \Delta_f G^0_{Cr,FCC} + G^{Cr}_{xs}$$

- Free energy of Ni^{2+} and Cr^{2+} in molten FLiBe uses a dilute solution energy function (MSTDB-TC)

$$G^0_{Ni^{2+}} = G^0_{Ni} + nFE^0_{Ni/Ni^{2+}}$$



Least-squares fit of Gibbs energy of Ni-Cr system from CALPHAD assessment

Kairos Power

MSTDB-TC: MOLTEN SALT CHEMISTRY APPLICATIONS FOR DEVELOPMENT OF THE KP FHR

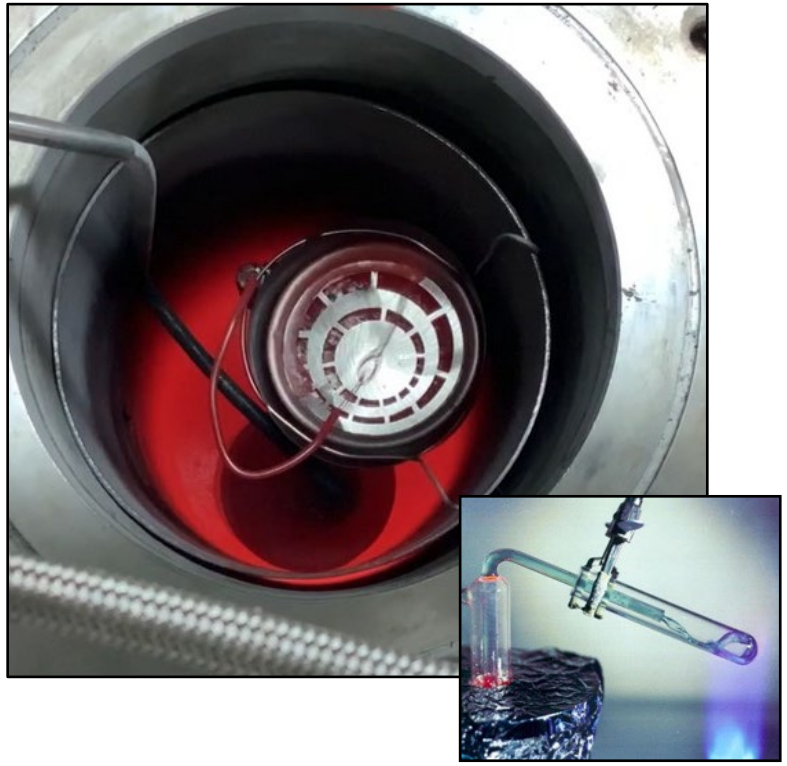
Kairos Power's mission is to enable the world's transition to clean energy, with the ultimate goal of dramatically improving people's quality of life while protecting the environment.

In order to achieve this mission, we must prioritize our efforts to focus on a clean energy technology that is *affordable* and *safe*.

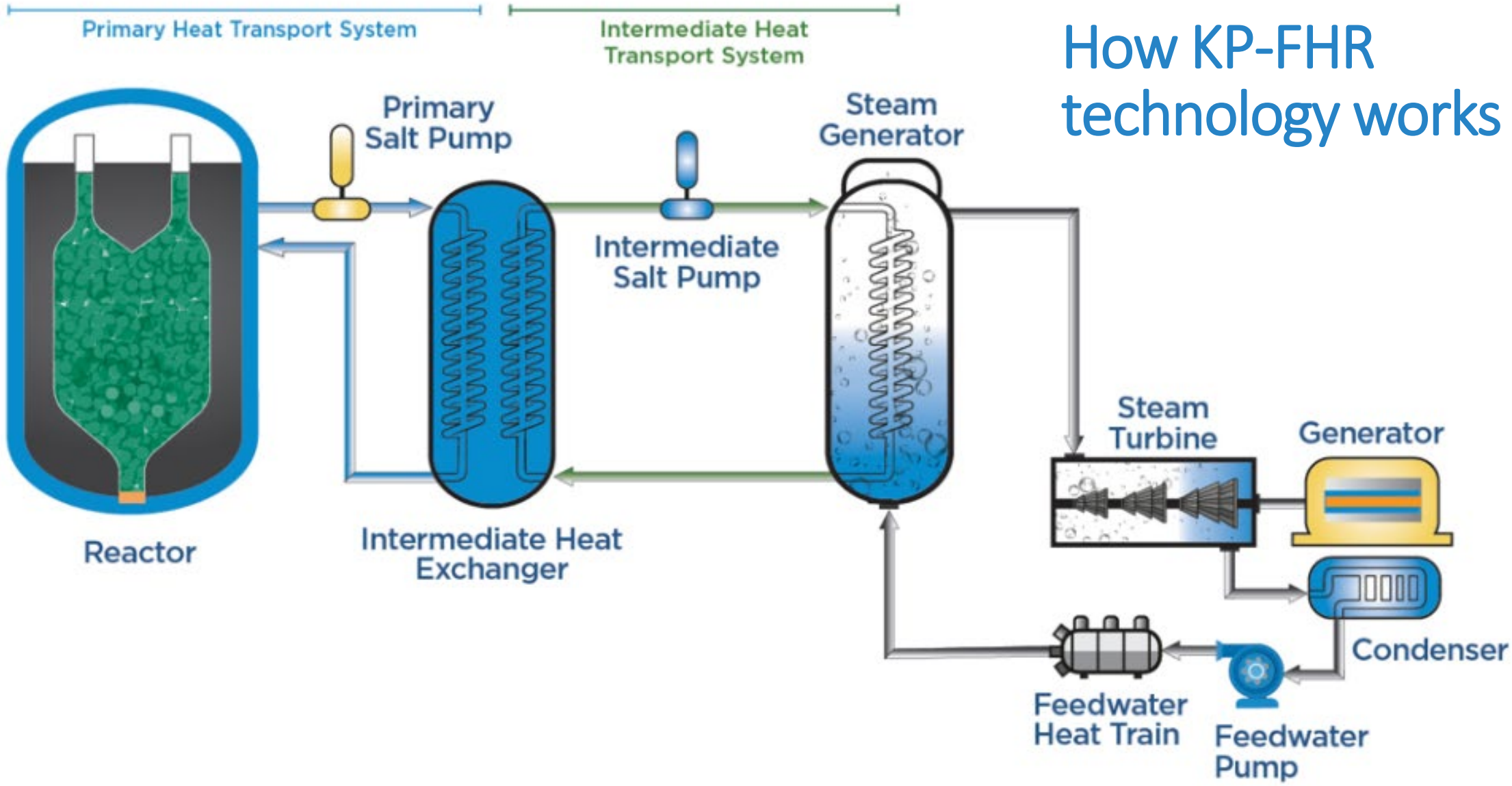
Fluoride Salt-Cooled High-Temperature Reactor (FHR) Technology Basis

Coated Particle Fuel
TRISO

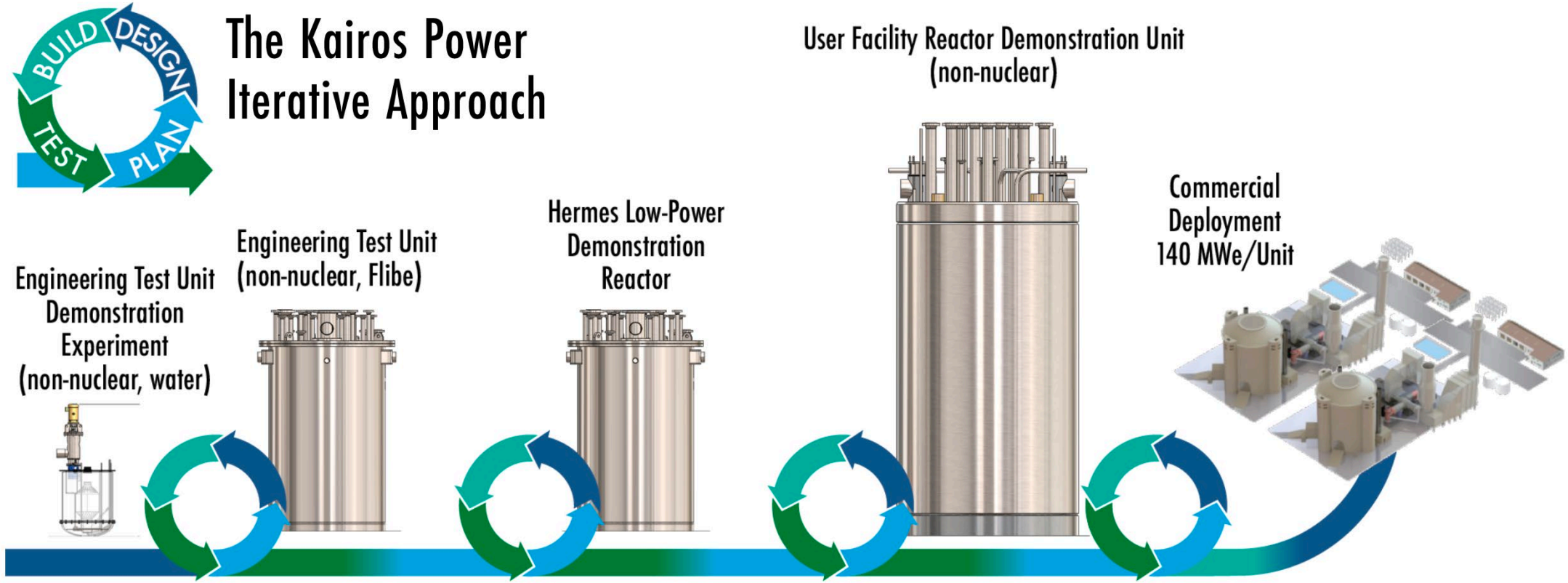
Liquid Fluoride Salt Coolant
Flibe ($2LiF\text{-}BeF_2$)



How KP-FHR technology works



A Paradigm Shift in Nuclear Development



Construction complete / hot commissioning in progress
November 2022

ETU Control Room
Albuquerque, NM

Argos Remote Control Room
Alameda, CA

Hermes Demonstration Reactor

Heritage Center K-33 Site / Oak Ridge, TN

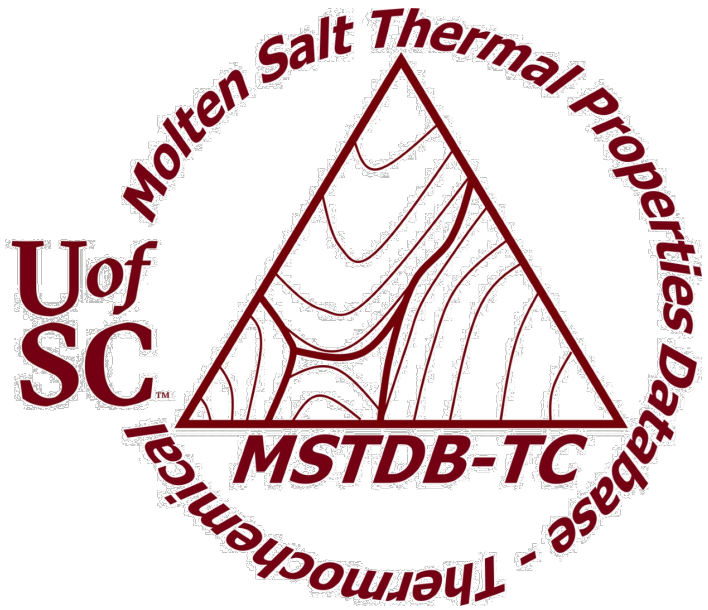
Hermes will ultimately demonstrate the U.S. aptitude to license an advanced reactor in a timely manner

How we use MSTDB

Provides multicomponent thermodynamic properties:

- chemical potentials
- species activities
- chemical state
- vapor pressures
- phase equilibria
- Etc.

At Kairos Power, we use this information in our modeling and simulation and processing



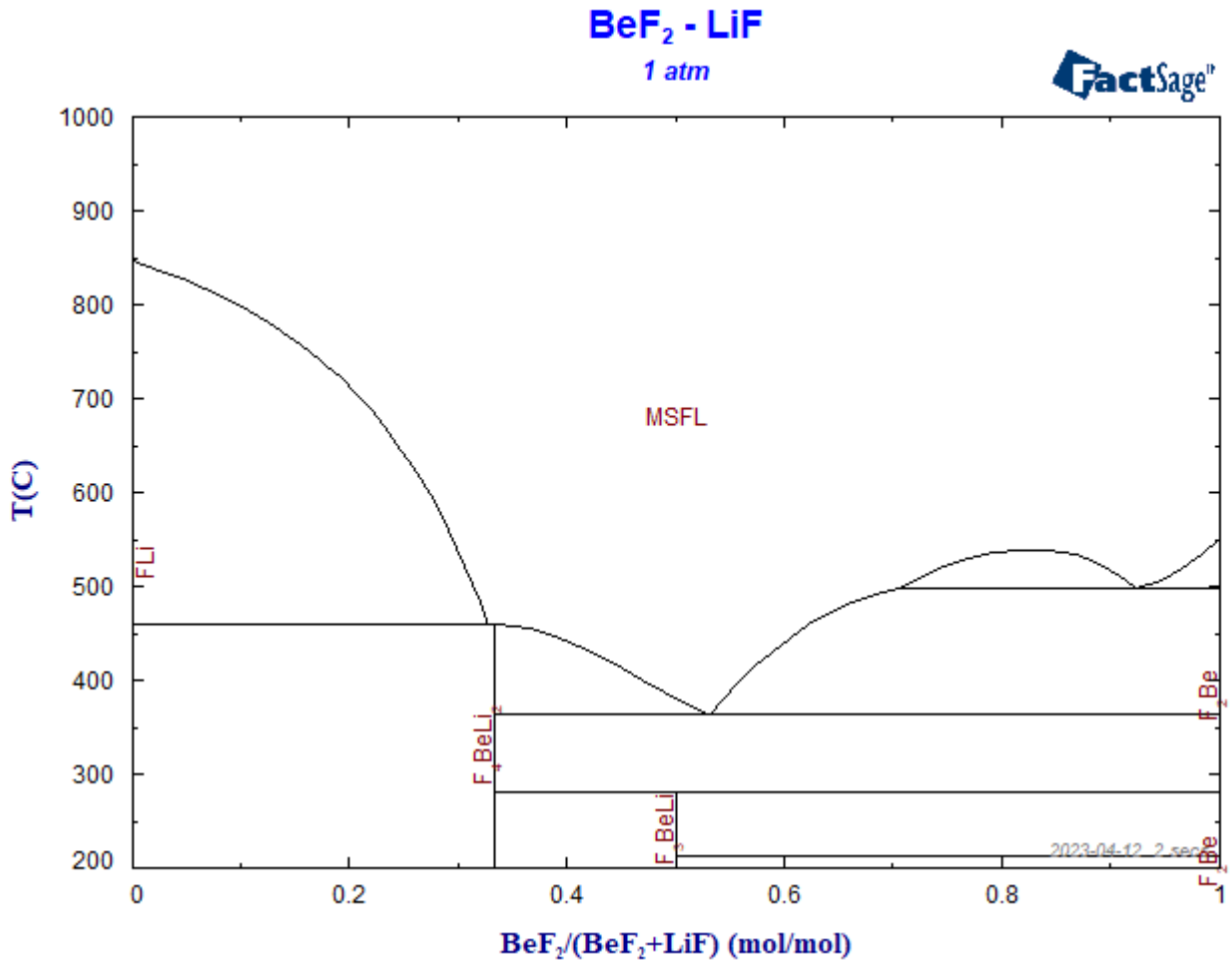
Kairos Power Commissions MSPP to Produce Coolant for High-Temperature Molten Salt Reactors

- Kairos Power has commissioned the **Molten Salt Purification Plant** (MSPP) in partnership with Materion Corporation
- MSPP will produce large quantities of high-purity fluoride salt coolant (Flibe) for the Engineering Test Unit and future hardware demonstrations
- **Confirms process to produce Flibe at industrial scale** and establishes commercial production
- Reduces risk in a critical path workstream to **achieve cost certainty for KP-FHR technology**
- Largest Flibe production facility ever built

Kairos Power | MATERION

MSPP is located at the Materion Campus in Elmore, Ohio

MSTDB-TC to support Flibe (0.667LiF-0.333BeF_2) production: The LiF-BeF_2 phase diagram



Thermodynamic inputs for design and safety case

- Inputs for safety models
  - Vapor pressures drive gas phase release
  - Chemical state determines vapor pressure
- Processing
- Performance and margins

These are the two big fundamental things I'm looking at

Equation 2.16 from the MELCOR Computer Code Manuals Vol 2: Reference Manual

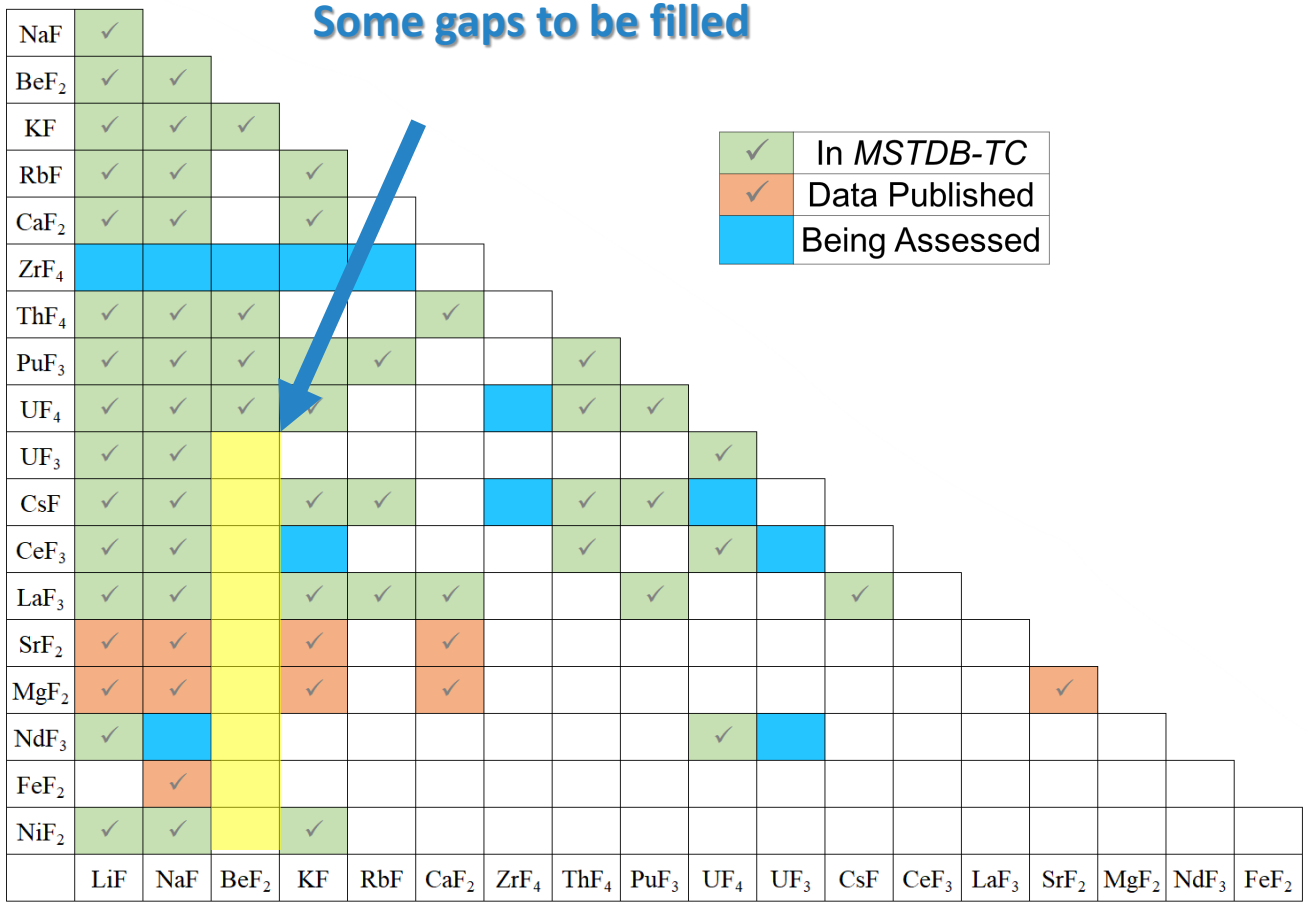
$$\frac{1}{\dot{m}_k} = \frac{D_{fuel} RT}{A_{fuel} Nu D_{k,gas} P_{k,eq}}$$

Equation 62 from Non-Proprietary version of the KP-FHR Mechanistic Source Term Methodology Topical Report

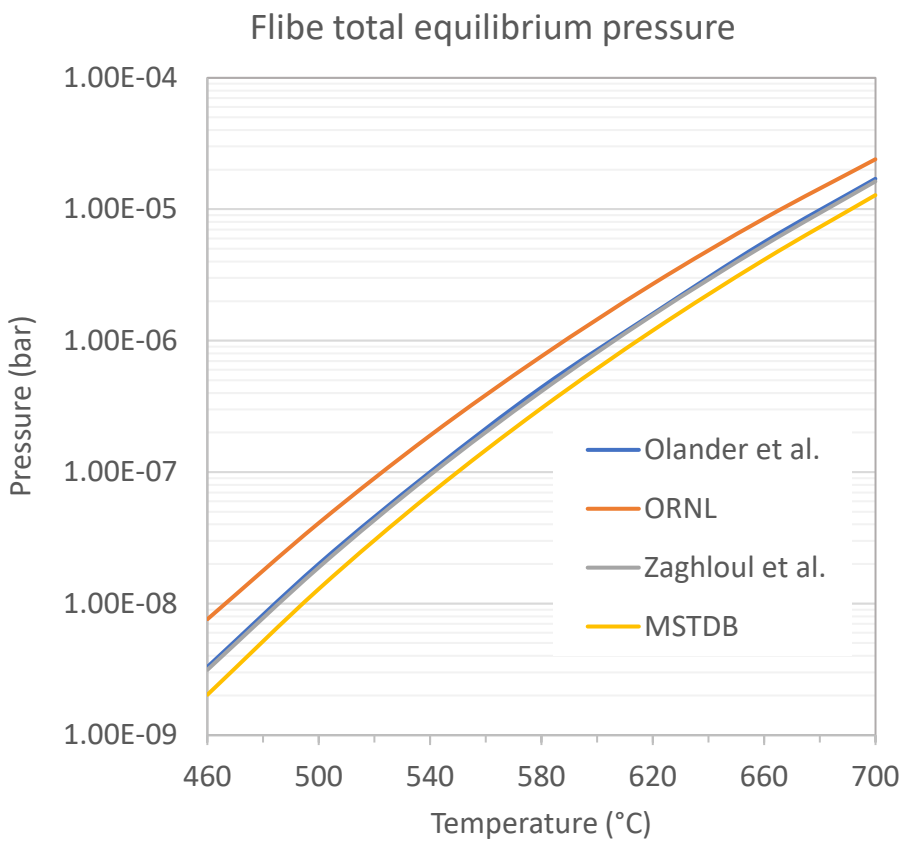
$$w_i = \frac{h_i p_i A}{RT}$$

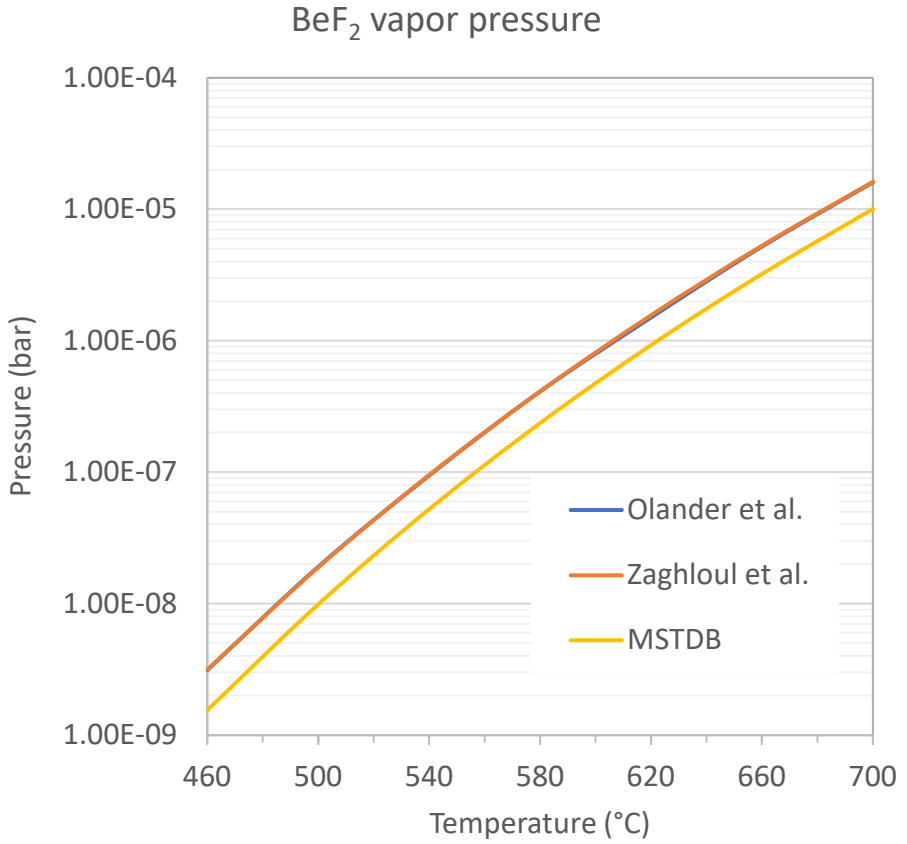
Current status of MSTDB-TC for the fluorides

- BeF2-LiF-NaF
- BeF2-LiF-PuF3
- BeF2-LiF-ThF4
- BeF2-LiF-UF4
- BeF2-NaF-PuF3
- 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-LiF-KF
- 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

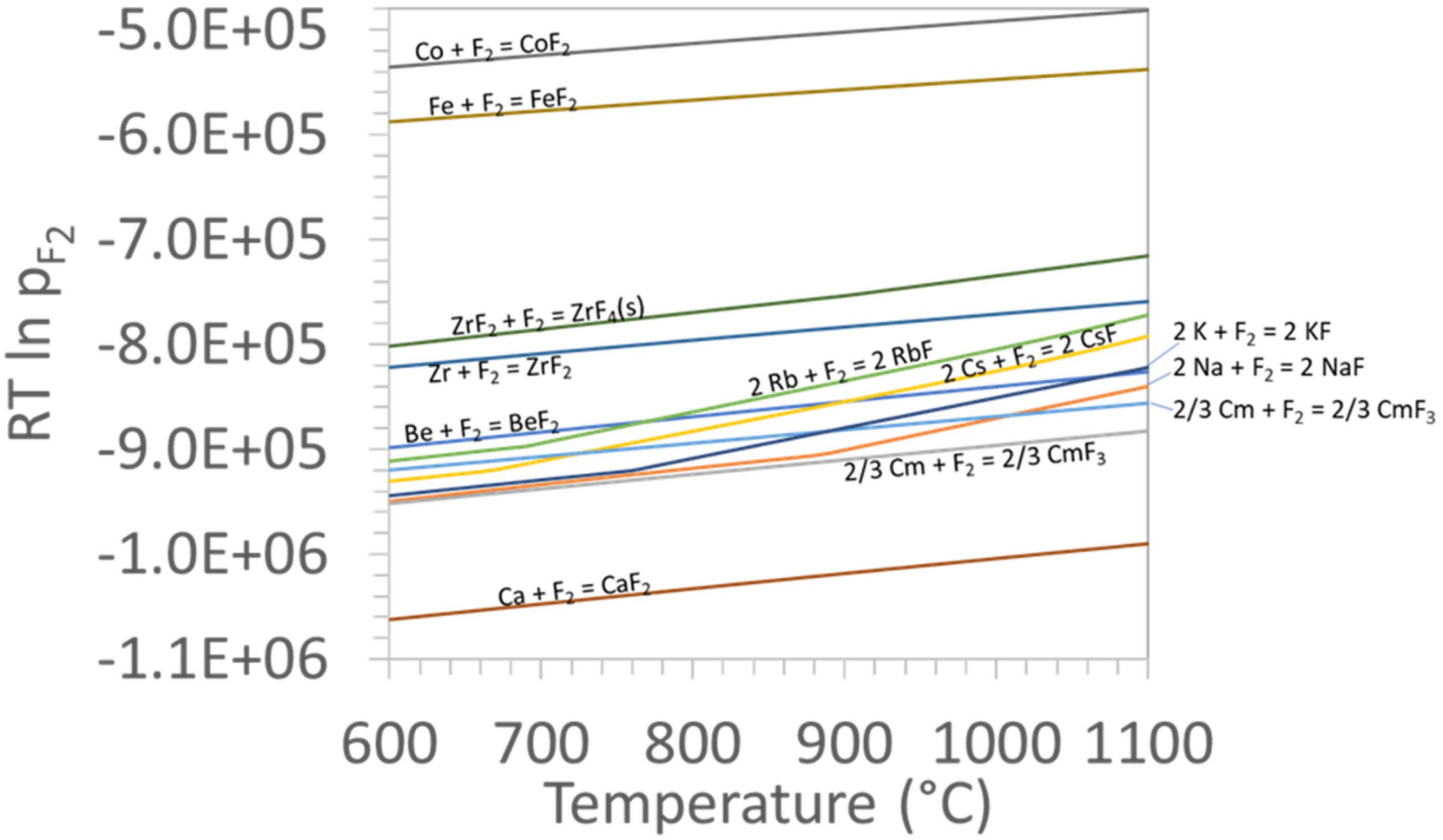


Vapor pressure of Flibe

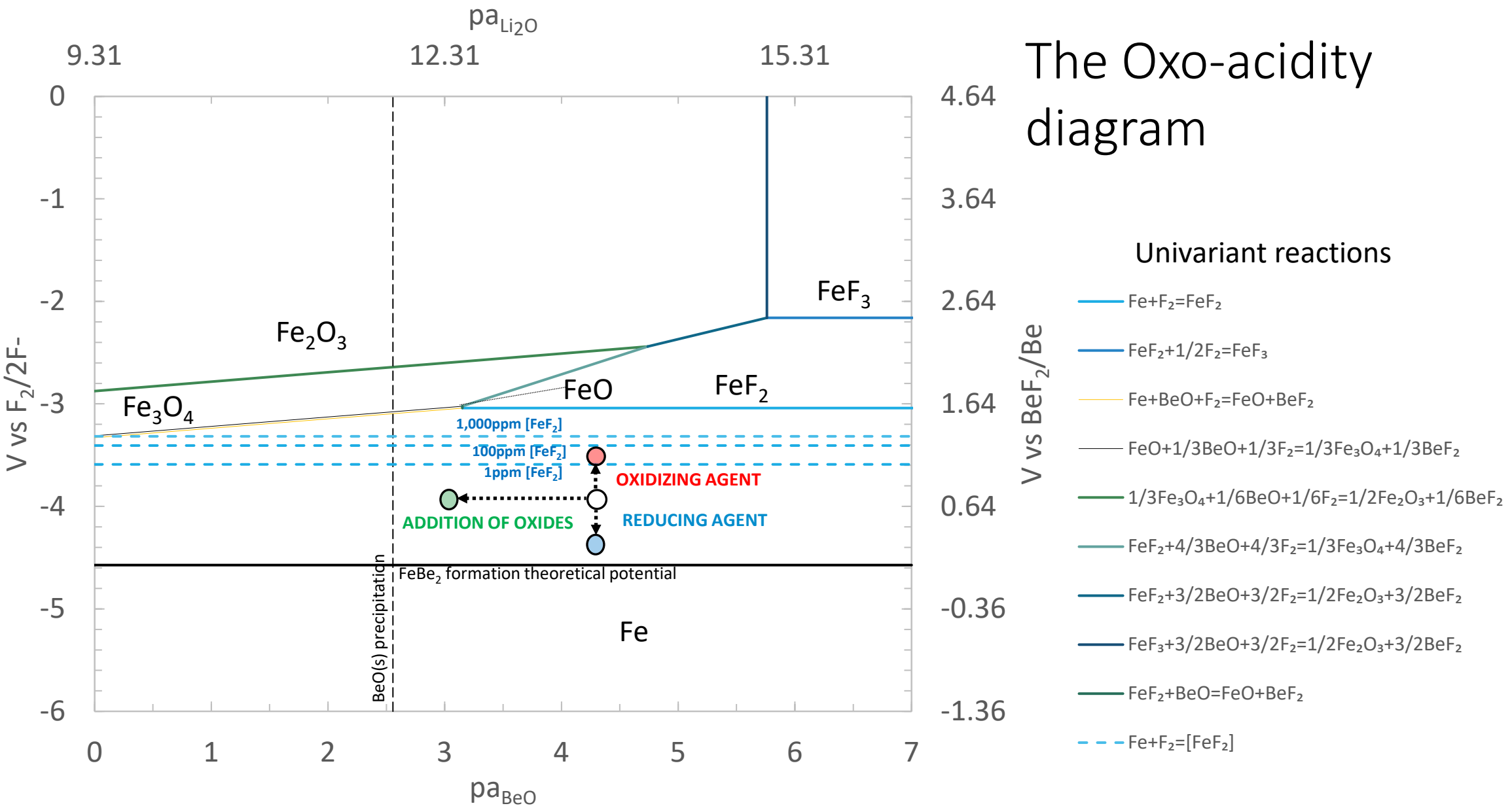




Fundamental aspects of molten salt chemistry



The Oxo-acidity diagram



Enabling the world's transition to clean energy

improving people's quality of life and protecting the environment

Our Commitment to Environmental Justice

- Mission driven
- Engaging and supporting local communities
- Diversity, equity and inclusion program
- Priority in building on brownfield sites
- High energy density / low land use

1 fuel pebble = 4 tons of coal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Oak Ridge, TN

OAK RIDGE National Laboratory

MSTDB-TP Development, Expansion, and Control Processes

Training/Workshop for the Molten Salt Thermal Properties Databases, April 25th 2023

Anthony Birri, birriah@ornl.gov

Nicholas Termini, Shane Henderson, N. Dianne Bull Ezell

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U.S. DEPARTMENT OF ENERGY

NEAMS Nuclear Energy Advanced Modeling and Simulation

Molten Salt Reactor PROGRAM

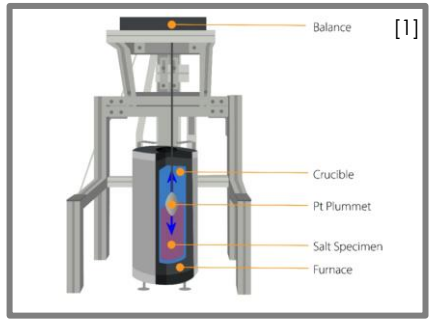
MSTDB-TP Overview

- 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 (more on this later)
- This list is constantly expanding. The data is based on the outputs of 140+ independent experimental studies in literature.

Experimental Measurement Techniques Considered: Density

- Density: Archimedean method, dilatometry method of maximum bubble pressure
- Viscosity: falling or rolling ball method, Rotational viscometry, coaxial cylinder technique, capillary viscometry
- Thermal conductivity: variable gap technique, coaxial cylinder technique, transient hot wire method, laser flash method
- Heat Capacity: DSC, drop calorimetry

Density



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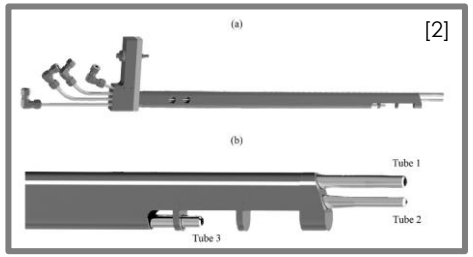

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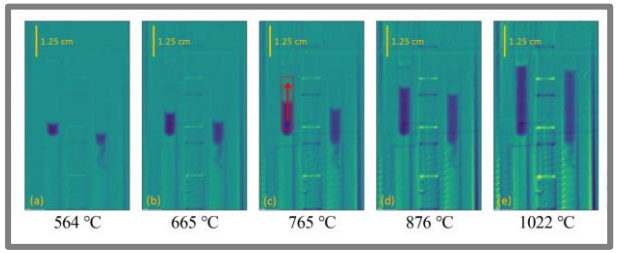

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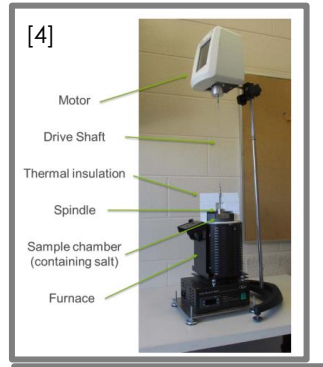
Viscosity



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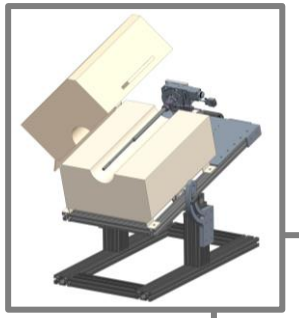

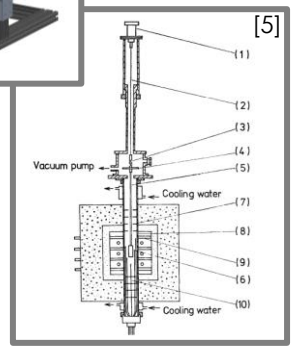

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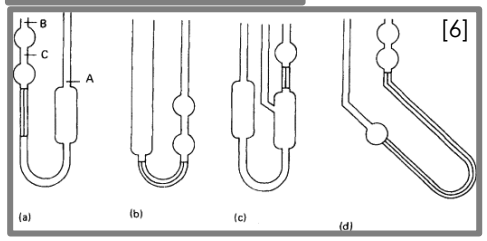

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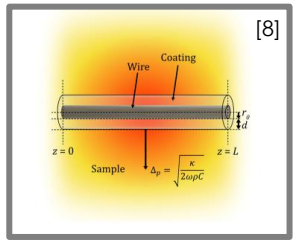
Thermal Conductivity



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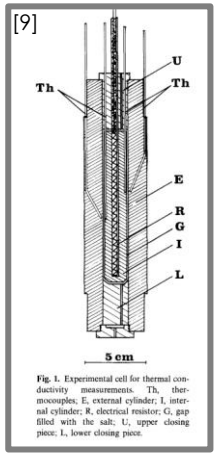

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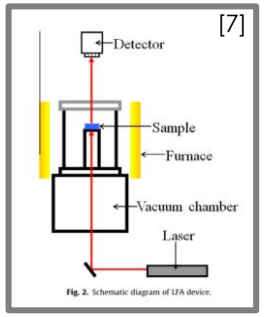

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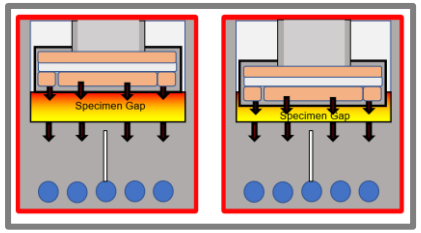
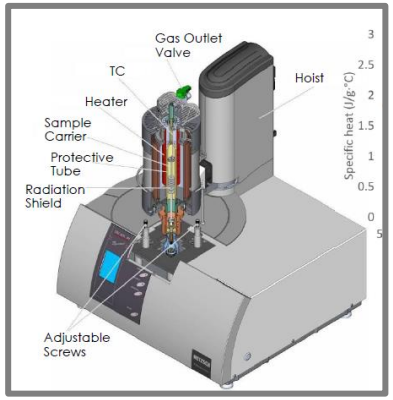
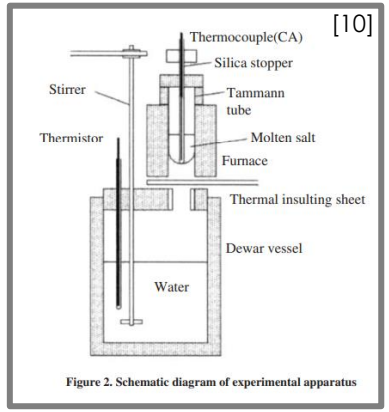


Heat Capacity





[10]

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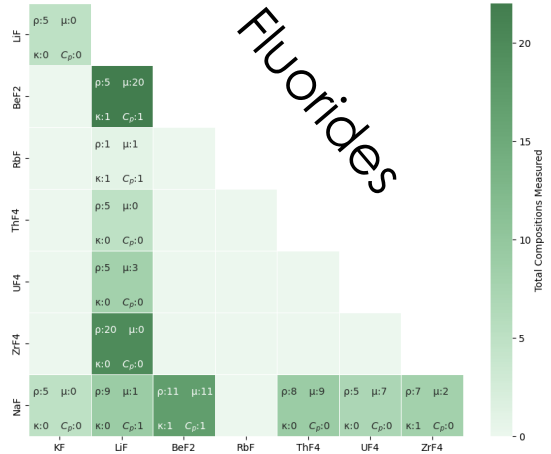
MSTDB-TP Expansion Efforts

- 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:



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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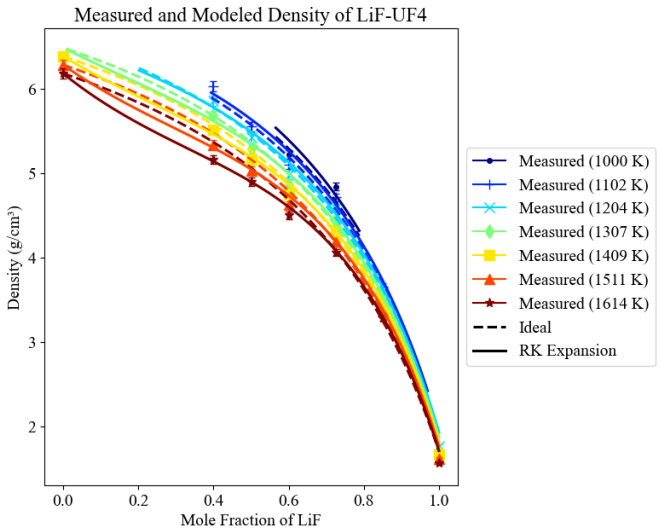
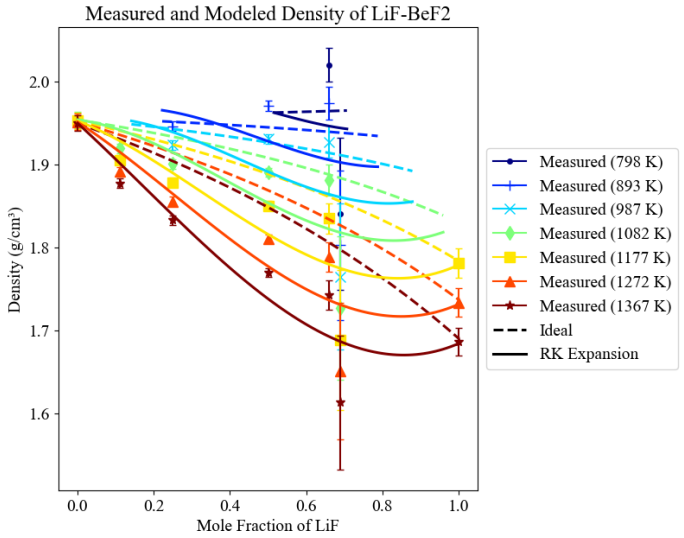
Redlich-Kister Density Models

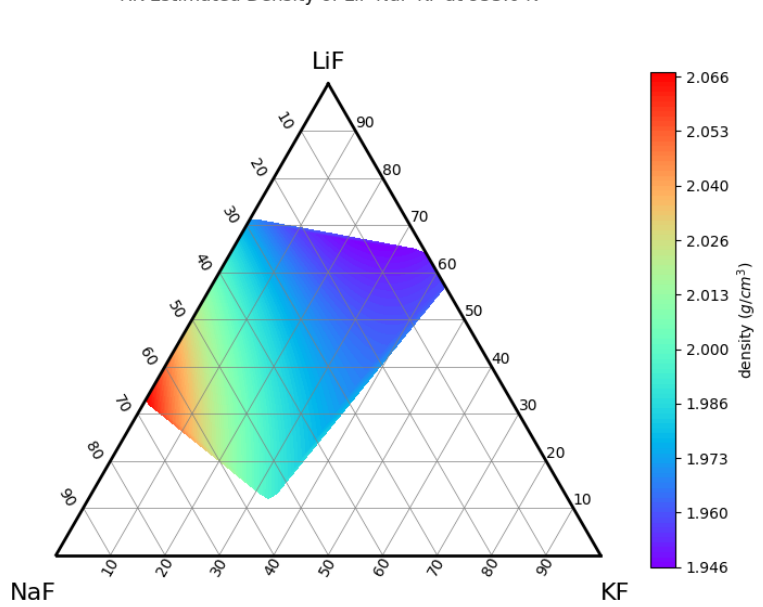
- Motivation: We can only make measurements across the national laboratories so fast
  - Time and funding is finite
  - There are countless possible pseudo-ternary+ systems which may be of interest, we cannot measure them all
- We therefore need estimation techniques to predict thermophysical properties of higher-order systems
  - Implementing Redlich-Kister framework with Muggianu extrapolation
  - We have validated the success of this technique with available density literature
- This is just one of many estimation techniques: we have chosen this technique specifically for rapid characterization of salt mixtures in the scope of MSTDB-TP

Pseudo-binary estimation examples





Pseudo-ternary estimation example

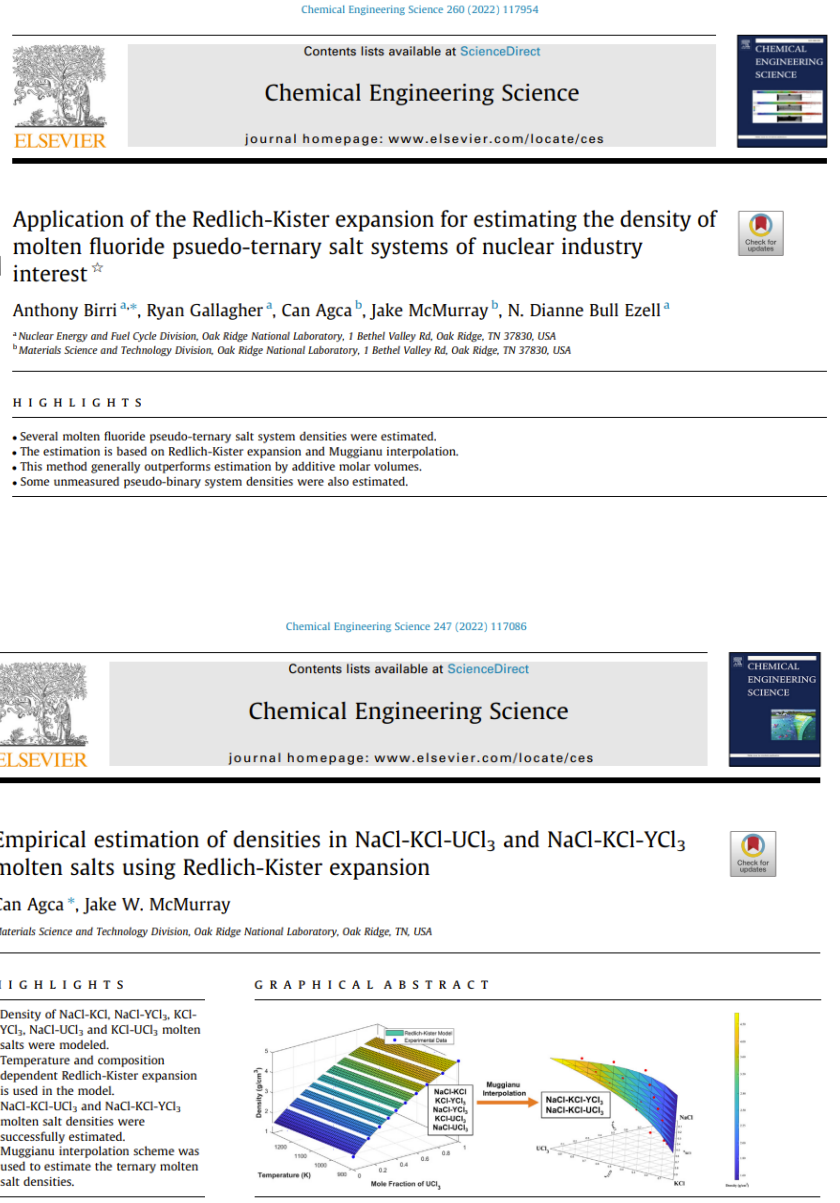


Redlich-Kister Density Models: Accessibility

- Redlich-Kister polynomials are temperature composition dependent, and follow a general formulation
  - Ideal term (based on additive molar volumes)
  - Non-ideal terms (interactions between each constituent)
- Interaction terms are tabulated and stored in the MSTDB-TP Gitlab project
  - Can be used as input in Saline to generate RK models
- Details about use of polynomials in previous publications

RK Parameters Generated for:

Fluorides	Chlorides
LiF-BeF2, LiF-KF, NaF-KF, NaF-LiF, NaF-ThF4, LiF-UF4, LiF-ZrF4, LiF-ThF4, NaF-ZrF4, NaF-UF4	LiCl-KCl, KCl-MgCl2, KCl-NaCl, KCl-UCl3, KCl-UCl4, NaCl-LiCl



Chemical Engineering Science 260 (2022) 117954

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 [a,*], Ryan Gallagher [a], Can Agca [b], Jake McMurray [b], N. Dianne Bull Ezell [a]

[a] Nuclear Energy and Fuel Cycle Division, Oak Ridge National Laboratory, 1 Bethel Valley Rd, Oak Ridge, TN 37830, USA
[b] Materials Science and Technology Division, Oak Ridge National Laboratory, 1 Bethel Valley Rd, Oak Ridge, TN 37830, USA

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.

Chemical Engineering Science 247 (2022) 117086

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

Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA

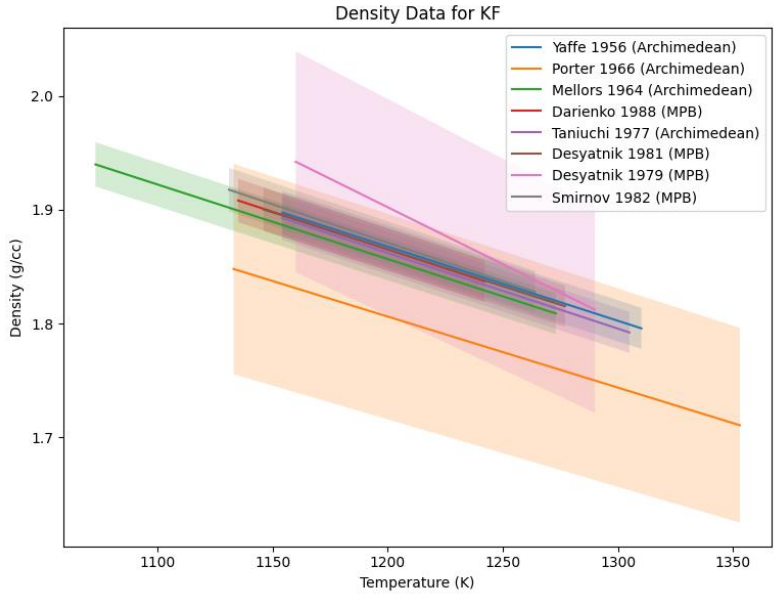
HIGHLIGHTS

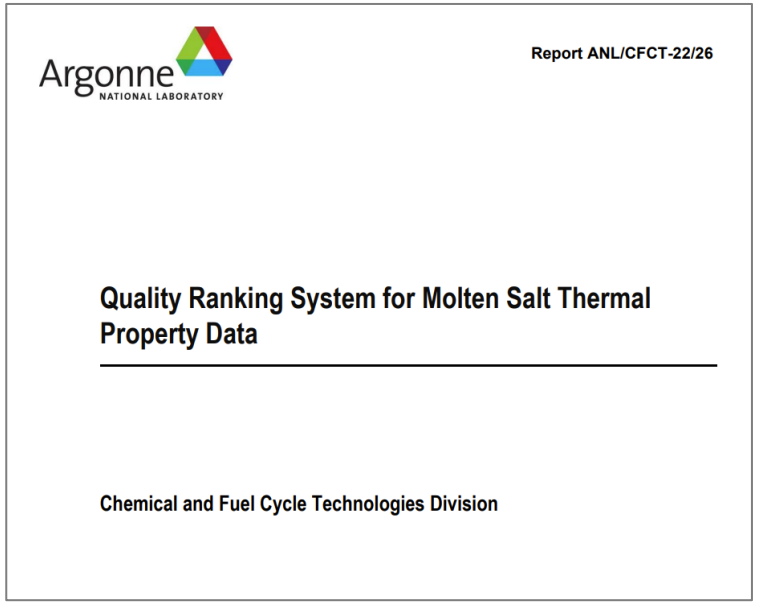
- Density of NaCl-KCl, NaCl-YCl_3, KCl-YCl_3, NaCl-UCl_3 and KCl-UCl_3 molten salts were modeled.
- Temperature and composition dependent Redlich-Kister expansion is used in the model.
- NaCl-KCl-UCl_3 and NaCl-KCl-YCl_3 molten salt densities were successfully estimated.
- Muggianu interpolation scheme was used to estimate the ternary molten salt densities.

GRAPHICAL ABSTRACT

Ongoing Effort: Quality Rankings, Methodology Assessment

- The MSR Campaign is funding the application of quality rankings to data in MSTDB-TP as well as duplicate data
  - Increased confidence in recommended data sets
  - Better characterization of uncertainty
  - Improved visibility about data selection process
- This ranking process will require tabulation and comparison of all duplicate data
  - When complete, these tabulations will be made available to database subscribers
- This effort will secondarily enable an assessment of methodologies used for thermophysical property measurement




Argonne NATIONAL LABORATORY

Report ANL/CFCT-22/26

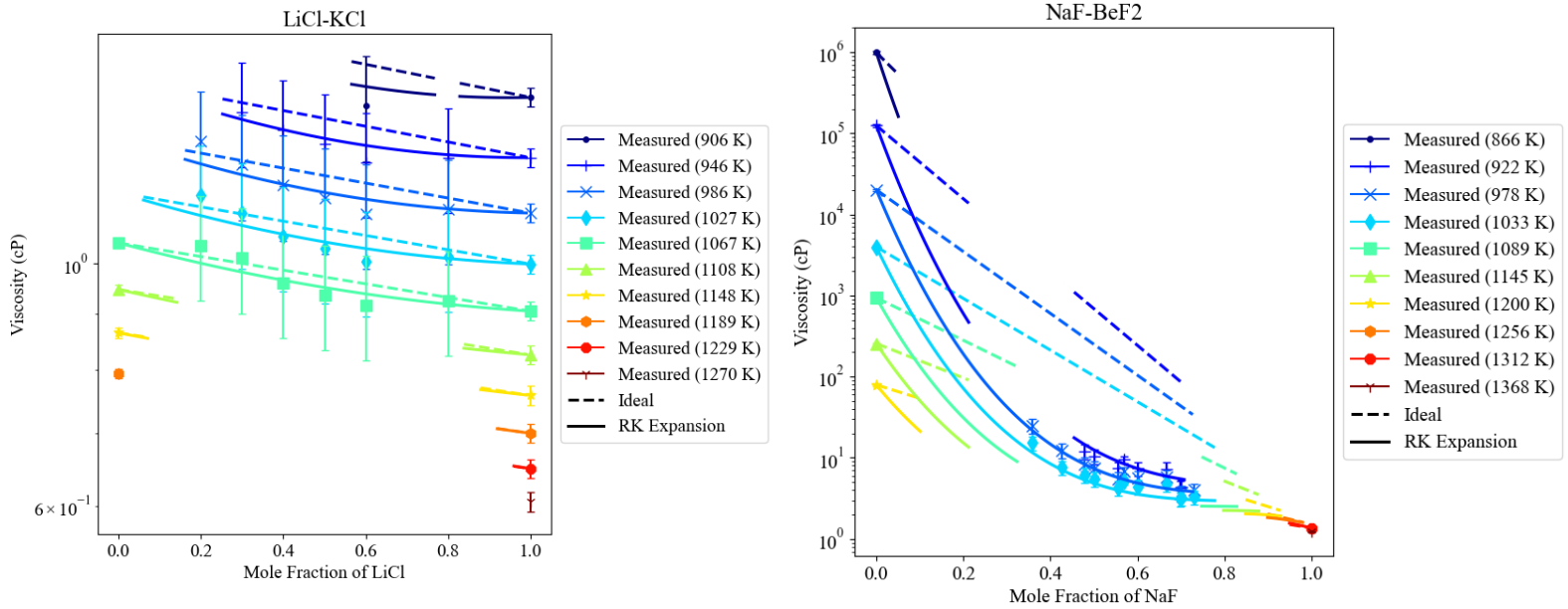
Quality Ranking System for Molten Salt Thermal Property Data

Chemical and Fuel Cycle Technologies Division

Ongoing Effort: Viscosity Estimation

- This FY we are tackling the challenging problem of creating estimation tools for viscosity estimation
- This 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



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How to get Access

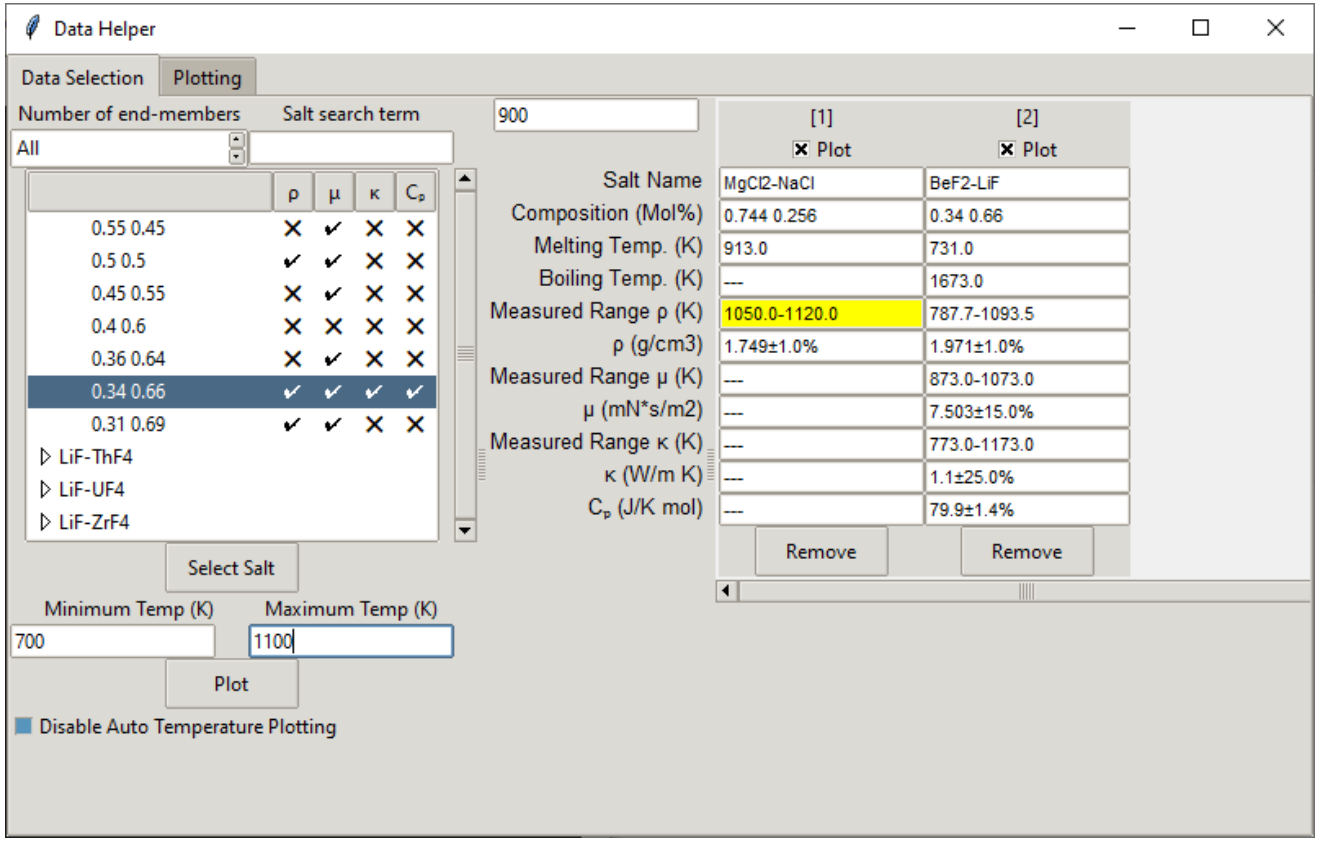
- The databases and associated documents are hosted on a publicly accessible, permission-protected server at Oak Ridge National Laboratory (ORNL): https://code.ornl.gov/neams/mstdb/. Access requires an ORNL XCAMS account and an MSTDB membership, which once granted will allow downloading of all files.

  - 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

User/Modeler Accessibility through GUI or API

- MSTDB-TP is a large, difficult to navigate .csv file
- We have developed accessibility options that will work for a variety of users
- 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



Questions?

Acknowledgements

This work is directly funded by the Nuclear Energy Advanced Modeling and Simulation (NEAMS) Program and the Advanced Reactors Program under the Office of Nuclear Energy

- The authors would like to acknowledge early contributors to the development of MSTDB-TP: Ryan Gallagher, Can Agca, and Jake McMurray
- The authors would like to thank Ted Besmann for guidance on MSTDB-TP development decisions
- The authors would like to acknowledge Melissa Rose for driving the Quality Assessment effort under the MSR campaign

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NEAMS Nuclear Energy Advanced Modeling and Simulation

Molten Salt Reactor PROGRAM

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Applications of MSTDB-TP in NEAMS for Modeling of MSRs

Bob Salko
Kyoung Lee

4/25/2023

ORNL is managed by UT-Battelle, LLC for the US Department of Energy

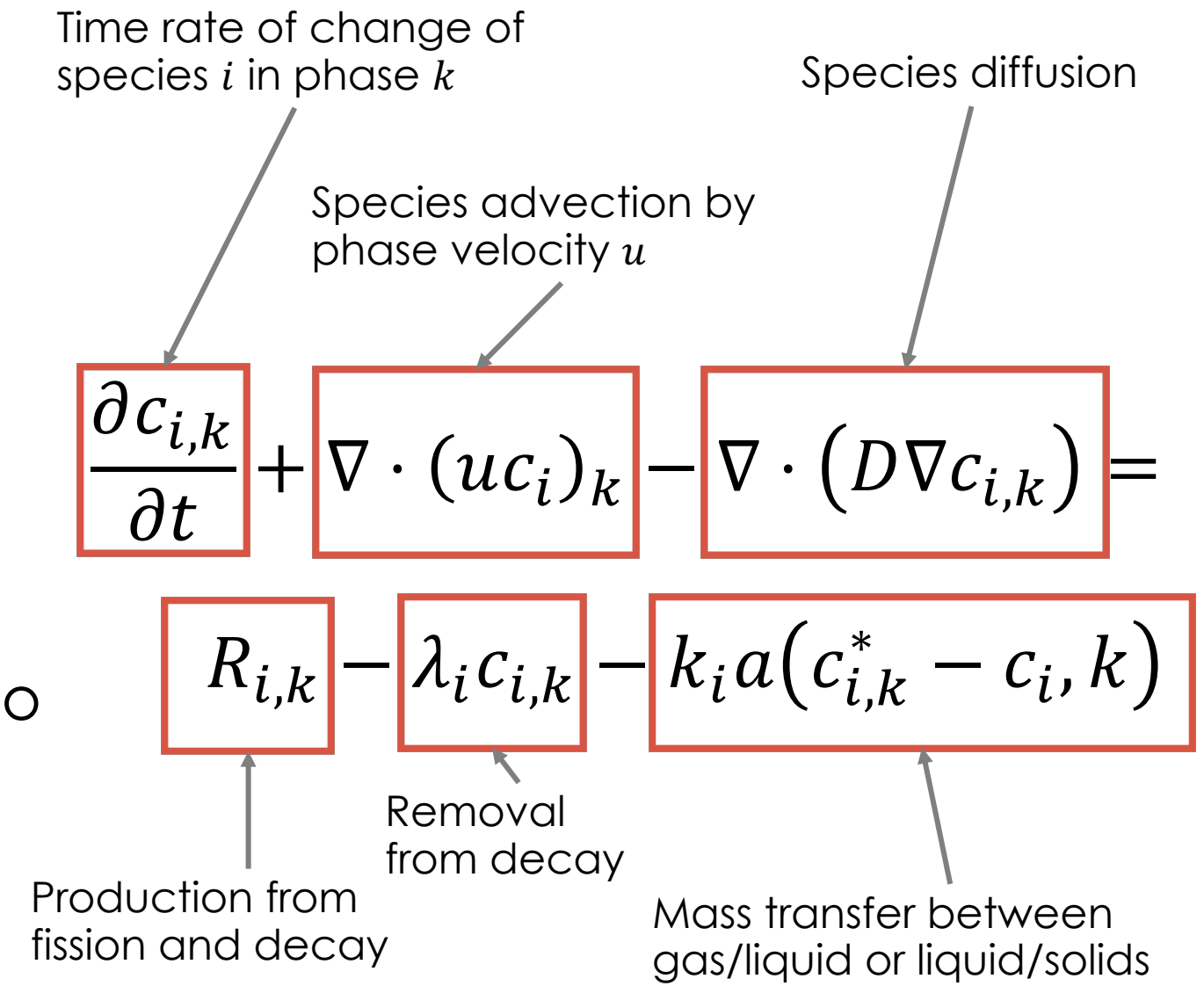
U.S. DEPARTMENT OF ENERGY

MSR modeling needs

- Liquid-fueled MSR designs pose unique modeling and simulation challenges
- NEAMS is developing new capabilities to model MSR designs with emphasis on:
  - Fuel depletion and composition
  - Tracking of delayed neutron precursors and impact on neutronic behavior
  - Generation and transport of fission products in the system
  - Behavior of entrained gas bubbles
- Specific NEAMS tools developed for MSR modeling include:
  - Mole: Mass transport
  - SAM: 1-D thermal-hydraulic behavior and gas transport
  - Griffin: Neutronics
  - Pronghorn: Porous media/Subchannel Thermal hydraulics and gas transport
  - NEK5000: High-fidelity CFD

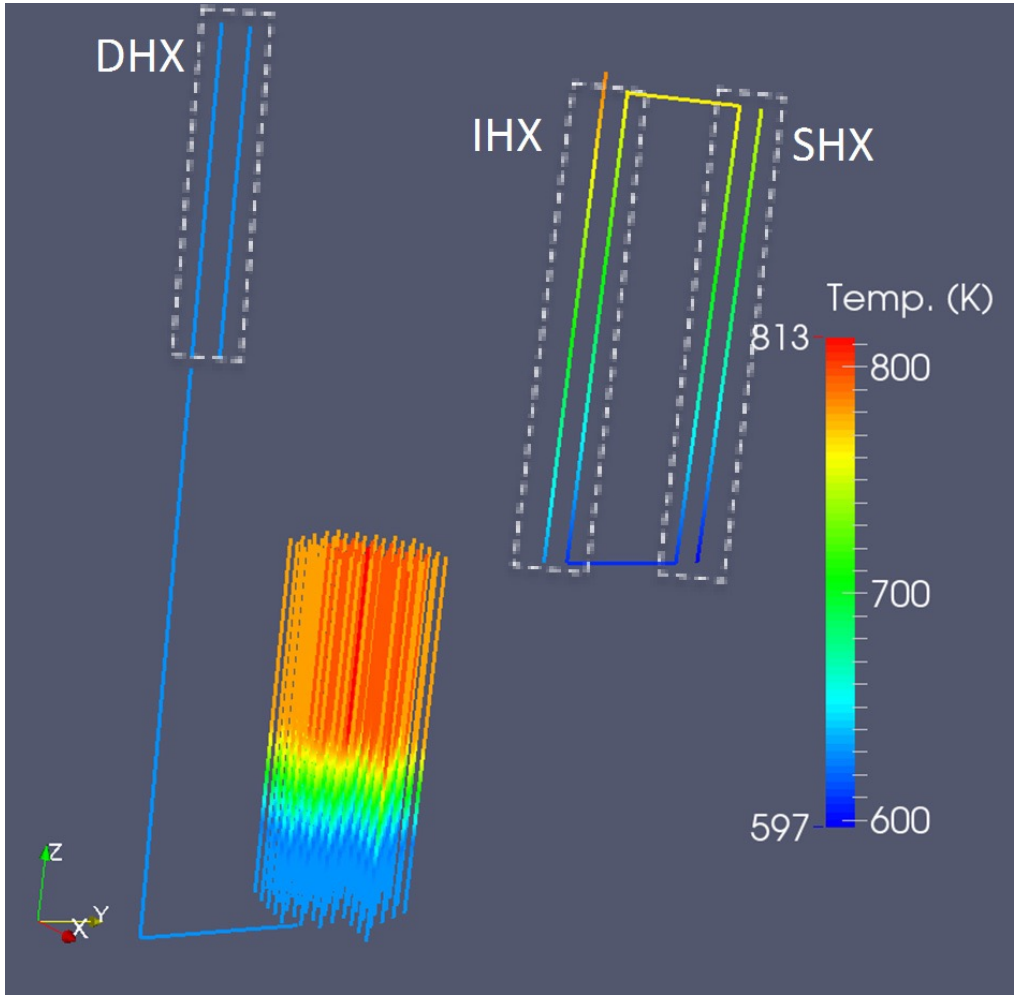
Mole

- Mole solves mass transport (convection/diffusion) of system of species/isotopes in the MSR system
- Species can exist in liquid or gas phase
- Species sources include:
  - Production from fission
  - Production from radioactive decay
  - Transfer between liquid/gas and liquid/solid surfaces
- Mole will be coupled to SAM to obtain required T/H parameters for mass transport calculation



SAM

- SAM is a system-scale thermal-hydraulic modeling tool written using the MOOSE framework and developed by ANL
- Solution of mass, momentum, and energy equations on 1D mesh
- Targeted applications include single-phase flow and heat transfer in advanced reactor systems
- Prediction of velocity, temperature in fluids and solids, and pressure during steady-state and transients



Temperature distribution predicted by SAM in the Advanced Burner Test Reactor

SAM gas transport model

- Presence of non-condensable gas phase in some MSR designs plays an important role in MSR behavior
  - Facilitates removal of fission gasses which can impact operational efficiency and safety (e.g., xenon and tritium)
  - Noble metals can affect heat exchanger efficiency and material corrosion and can also interact with entrained gases
- Model added to SAM to capture gas transport and local behavior
- Results in prediction of local gas void, bubble velocity, and bubble diameter/interfacial area

$$\frac{\partial(\alpha\rho_g)}{\partial t} + \nabla \cdot (\alpha\rho_g u_g) = S$$

Gas conservation equation added to SAM

$$u_g = C_0 u_l + u_{gj}$$

Gas velocity calculated using drift-flux model, where gas distribution is dependent on salt viscosity and drift velocity is dependent on surface tension

$$We = \frac{\rho_l u_r^2 d}{\sigma}$$

Bubble diameter d depends on surface surface tension and impacts interfacial area calculation

Saline integration

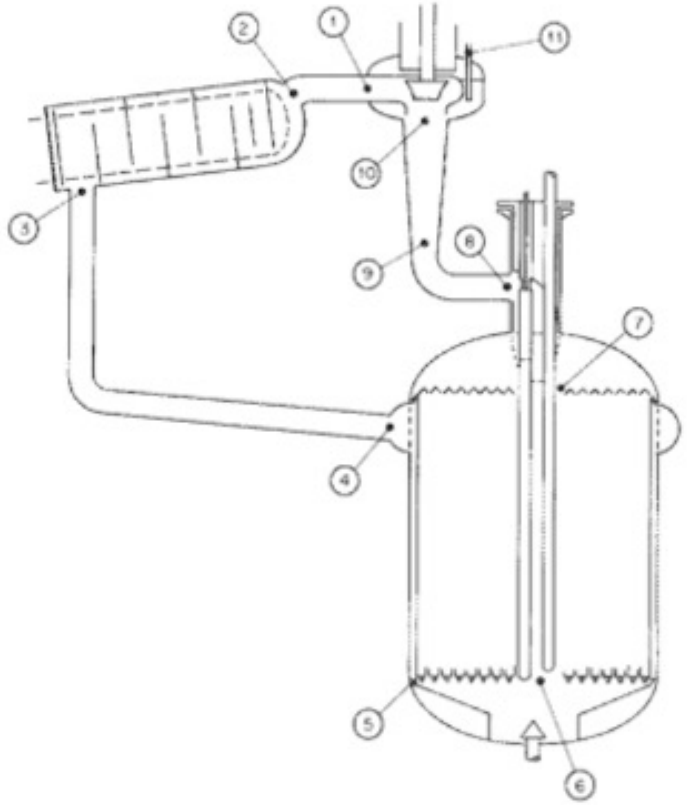
- Gas and species transport models depend on accurate thermophysical and thermochemical properties with quantified uncertainties
- Saline provides C interface to MSTDB-TP properties for many salt compositions that is easily incorporated into SAM, Mole, and other MOOSE-based codes
- Saline integrated into the MOOSE fluid properties module for use by all MOOSE codes
- Option for using Saline added to SAM and Mole

```
[EOS]
  [./eos]
    type = SalineInterface
    comp_name = "LiF-NaF-KF"
    comp_val = "0.465-0.115-0.42"
  [../]
[]
```

SalineInterface can be selected as an eos object in SAM with both salt composition specified

Molten Salt Reactor Experiment (MSRE) modeling

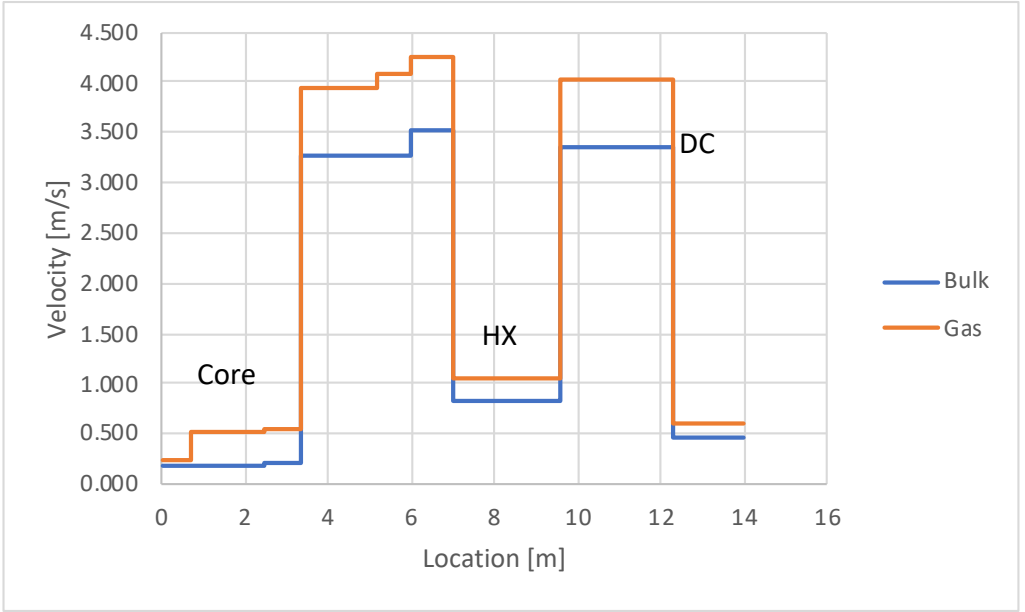
- MSRE was operated at Oak Ridge National Laboratory from 1965-1969
- Operation led to insights related to fission product behavior, migration, and impact of gas entrainment
  - Fission products include "salt-seekers", which stay in solution, and noble metals, which migrate to graphite and metal surfaces as well as the gas phase
  - Noble gases like Kr and Xe migrate to offgas system
- This system was modeled in both Mole and SAM

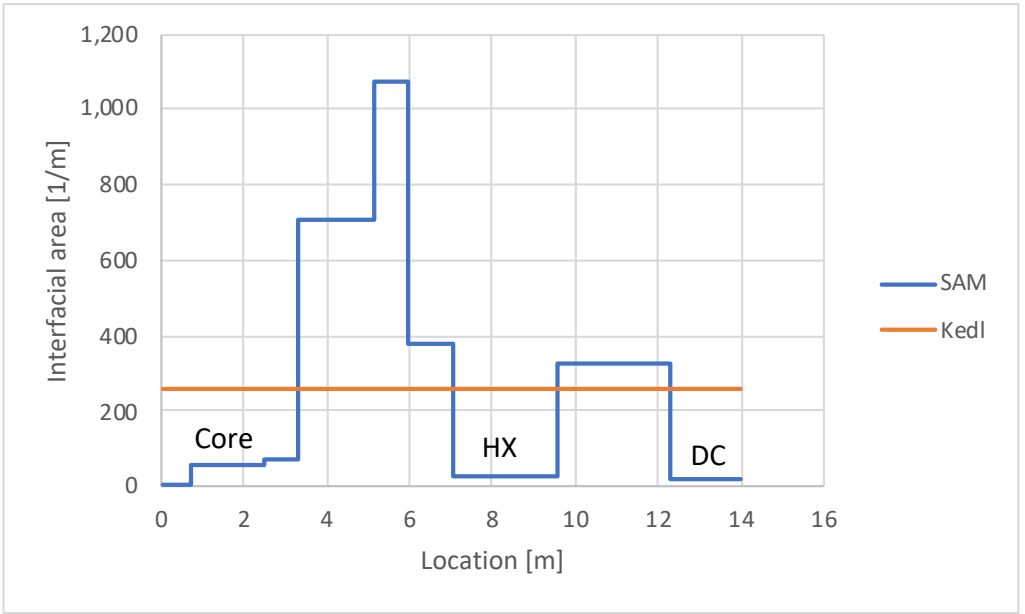


Schematic of the MSRE facility

MSRE modeling

- SAM model provides prediction of gas velocity and gas surface area distribution in the system
- Analytical model proposed by Kedl assumes constant interfacial area based on assumed bubble diameter and system gas holdup
- Phase slip and local pressure can lead to changes in interfacial area and mass transfer

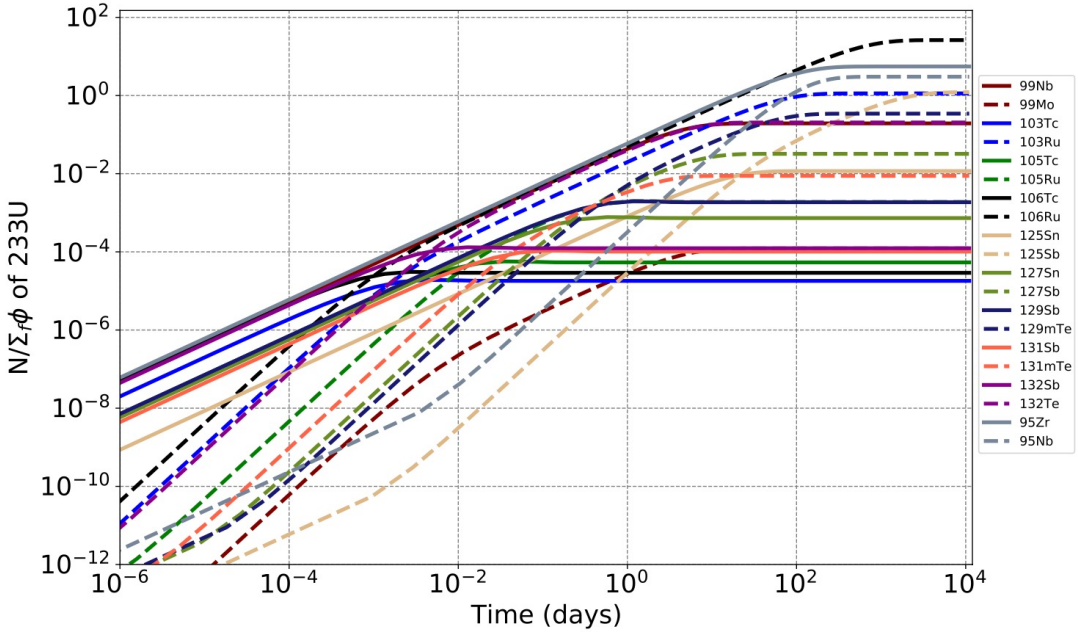




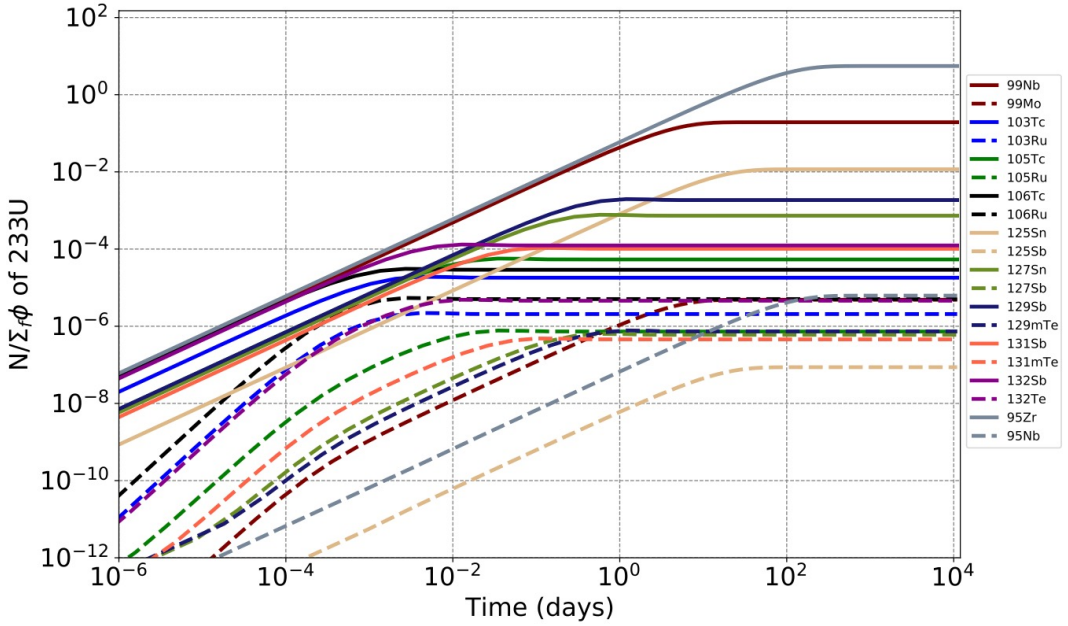
OAK RIDGE National Laboratory

MSRE modeling

- Mole predicts steady-state concentration of noble metals of interest in MSRE
- Current results assume Interfacial area predicted by Kedl (not yet coupled to SAM)
- Prediction will be used to determine fission product deposition and removal from the system



No transfer to wall or gas



Transfer to wall/gas enabled

Conclusion

- NEAMS is developing tools for multiphysics simulation of advanced reactor systems including MSRs
- SAM and Mole are being developed for modeling of the mass transport problem unique to liquid-fueled MSR designs
- A gas transport model was added to SAM to provide Mole interfacial area data for the mass transport solution
- Saline was integrated into MOOSE and made available to both SAM and Mole
- A demonstration was performed for MSRE mass transport showing the importance of capturing local T/H behavior and consideration of gas and solid mass transport

Future work

- SAM and Mole will be coupled for prediction of mass transport in MSRE and other designs
- The SAM gas transport model is being further validated against available data
- As new data becomes available, new models may be developed to capture bubble dynamics (e.g., breakup, dissolution)
- Mole is developing off-gas system for high volatile gas

Sensitivity Analysis of Thermophysical Properties of Molten Salts using a MSDR Model in TRANSFORM

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Outline

- Goals
- Property Perturbations
- Methodology
- Results
- Conclusion

Goals

- Investigate uncertainties in molten salt thermophysical properties that could be a risk to licensing
  - Density, thermal conductivity, heat capacity, and viscosity
  - Steady state and transient scenarios
- Determine uncertainty values for all four thermophysical properties
- Determine if measurements need to be refined
- Determine if thermophysical properties need to be known with less uncertainty

Perturbation of Properties

Property	Nominal Value/Equation	Uncertainty	Intermediate Perturbations
Density (kg/m^3)	3785-0.373×T(K)	10%	5%
Viscosity ($kg/(s \cdot m)$)	$1.09e^{-4} \times \exp(4090/T(K))$	30%	20%, 10%
Heat Capacity ($J/(kg \cdot K)$)	1340	25%	15%, 5%
Thermal Conductivity ($W/(m^2 \cdot K)$)	1.3	30%	20%, 10%

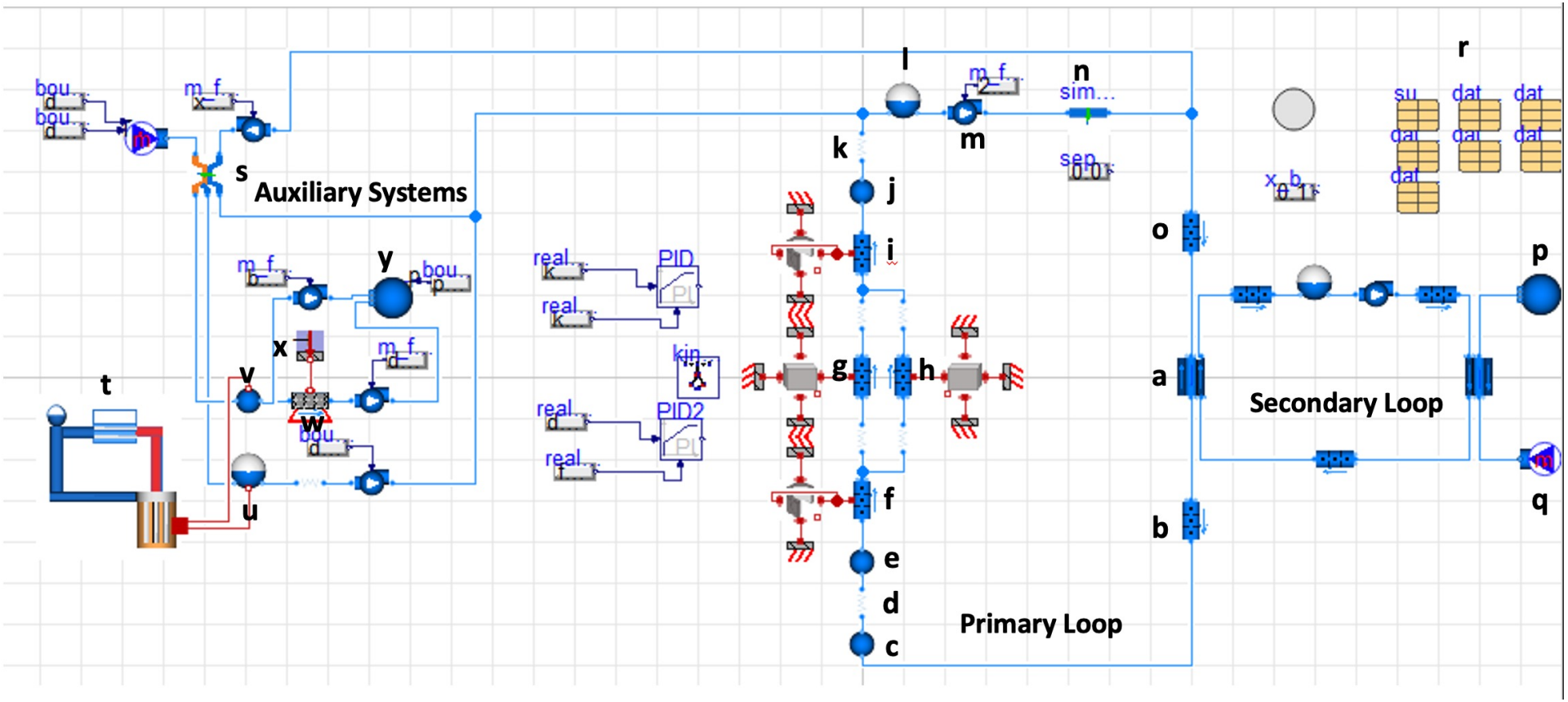
Methodology

- Modelica
- TRANSFORM
- Dymola

Model Information

- 750 MW_{th}
- $LiF\text{-}BeF_2\text{-}ThF_4\text{-}UF_4$
  - (71.5-16.0-12.0-0.5 mole%)
- $LiF\text{-}BeF_2$ (67-33 mole%)

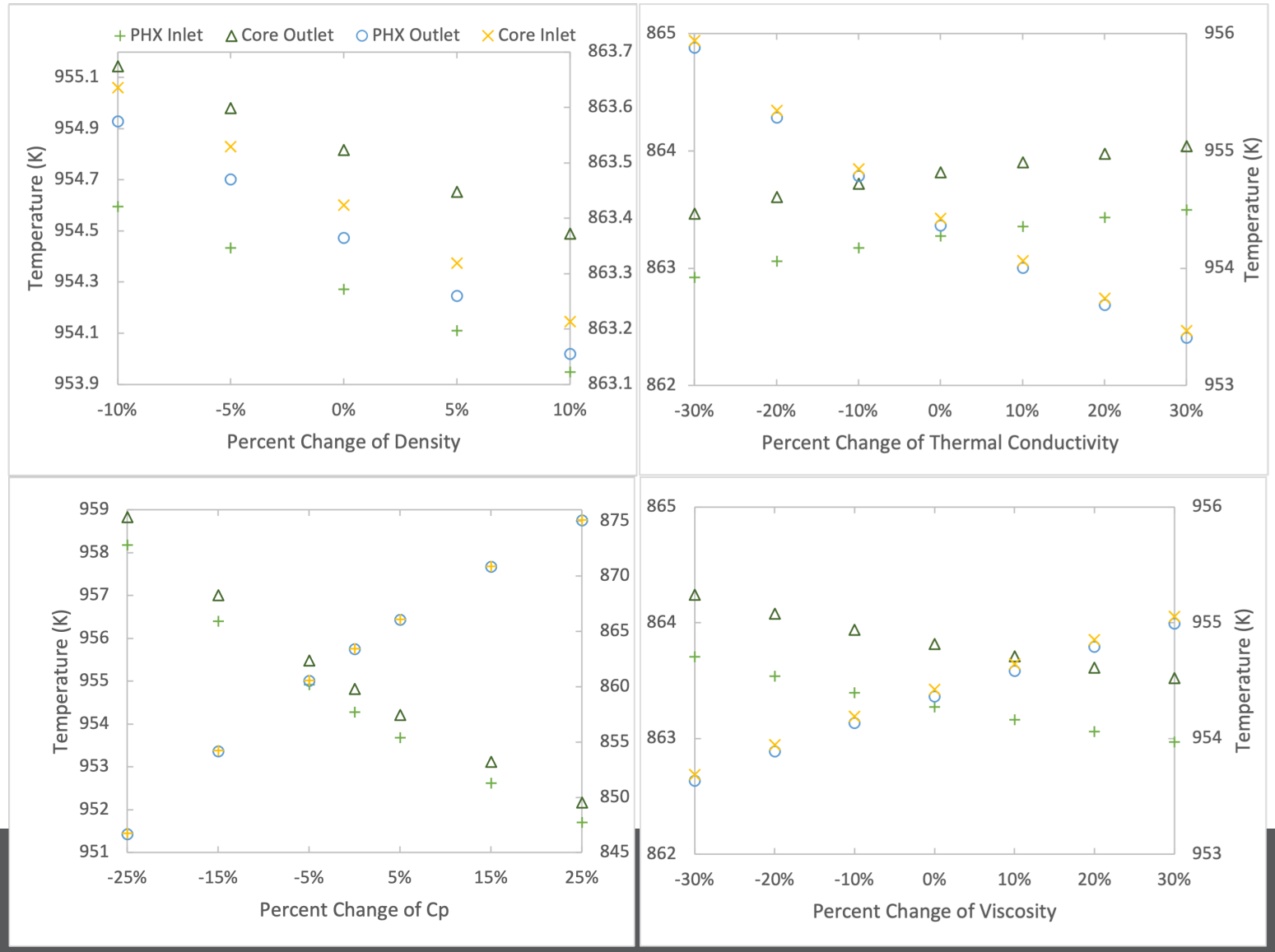
TRANSFORM Model



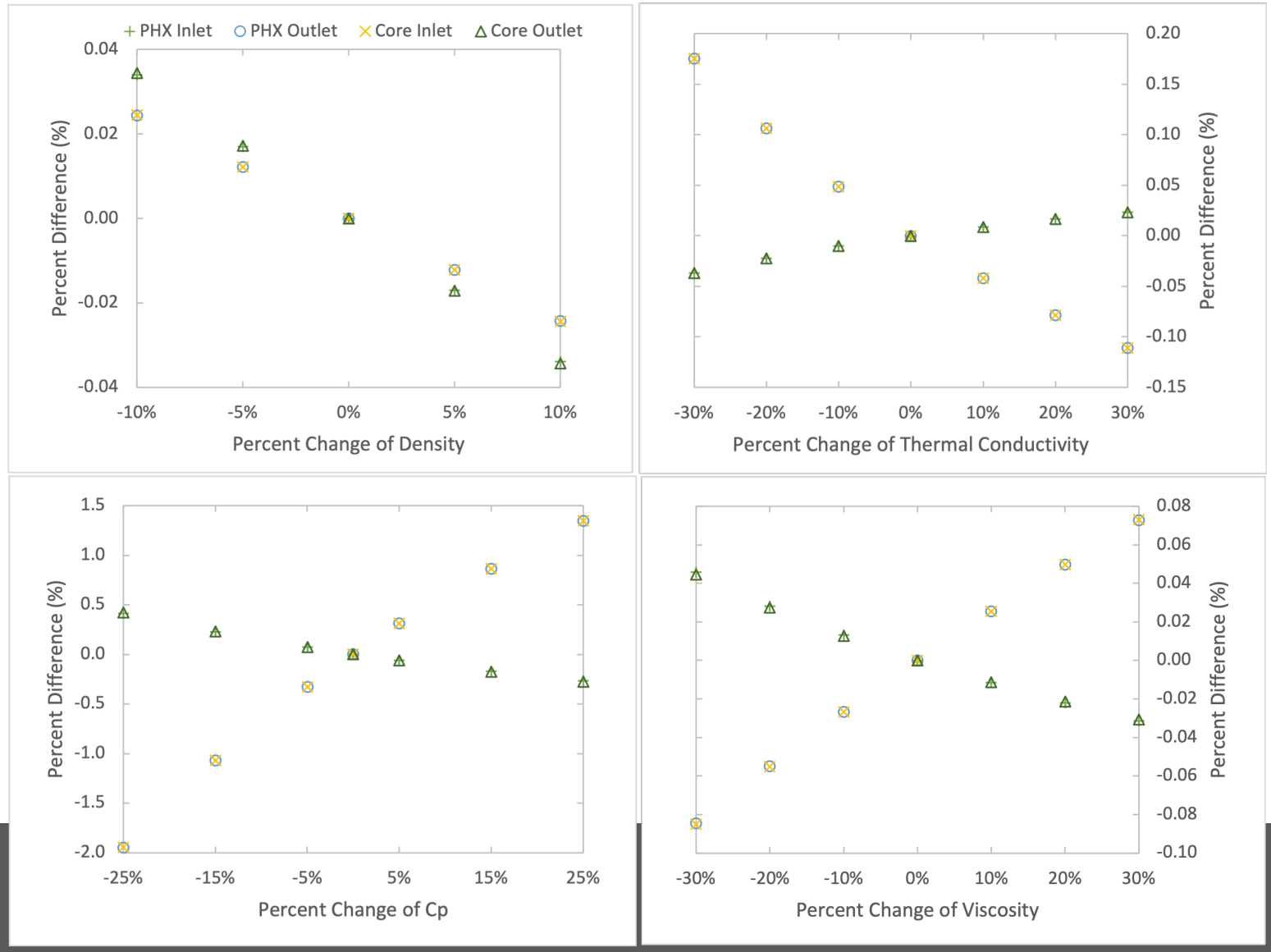
Results

- Steady State
  - Plots of temperature and percent difference
- Reactivity Insertion
- Buildup
- Varying Two Properties at a Time

Steady State Results



Steady State Results



Results

- Steady State
- Reactivity Insertion
  - Plots of temperature and percent difference
- Buildup
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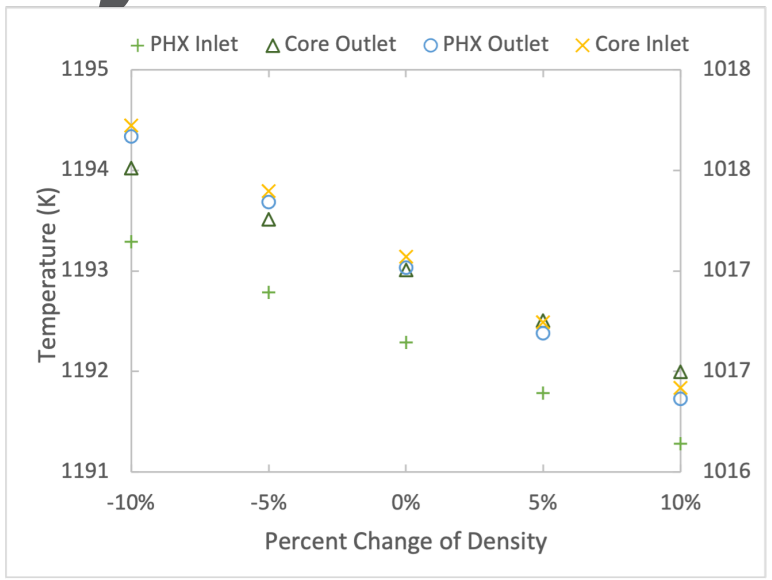
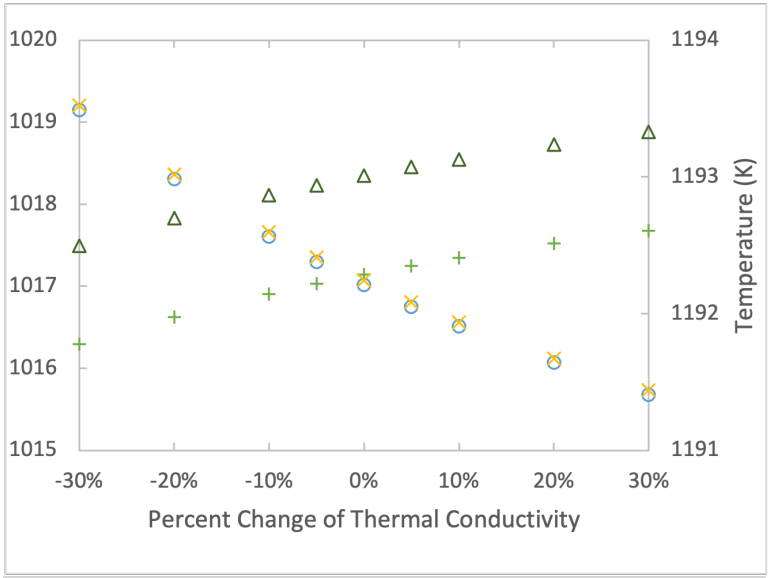
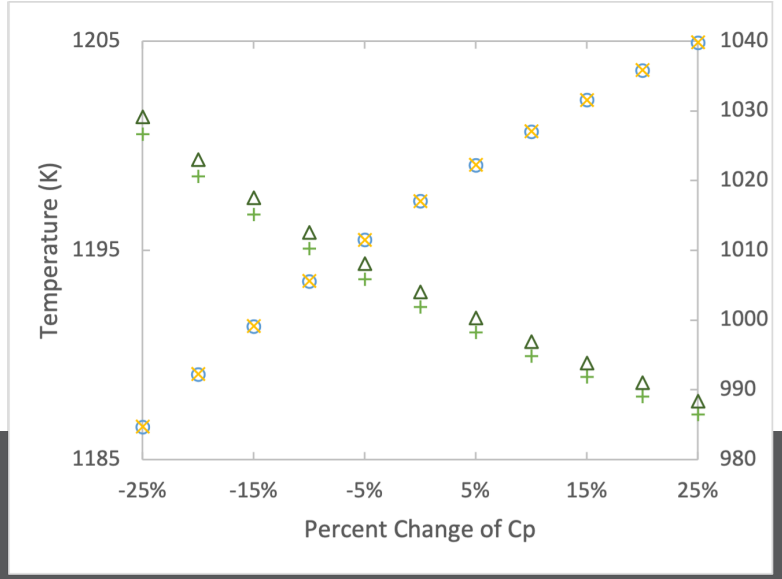
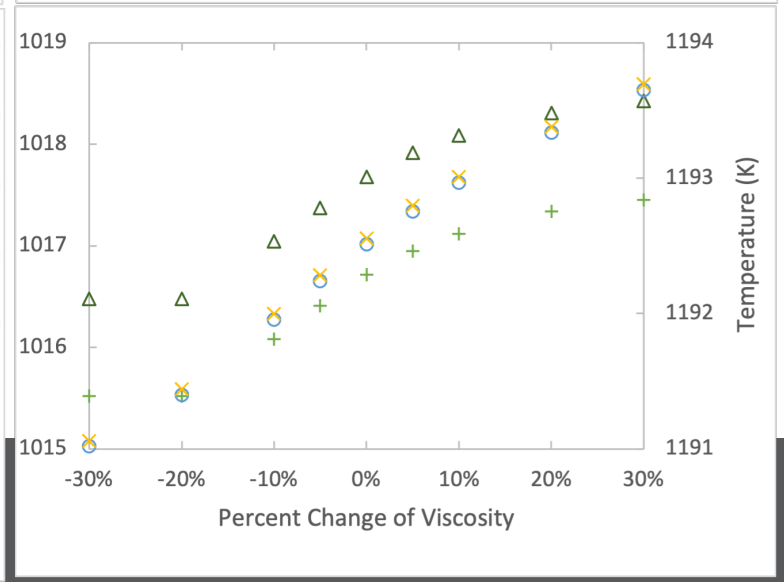
Reactivity Insertion Results

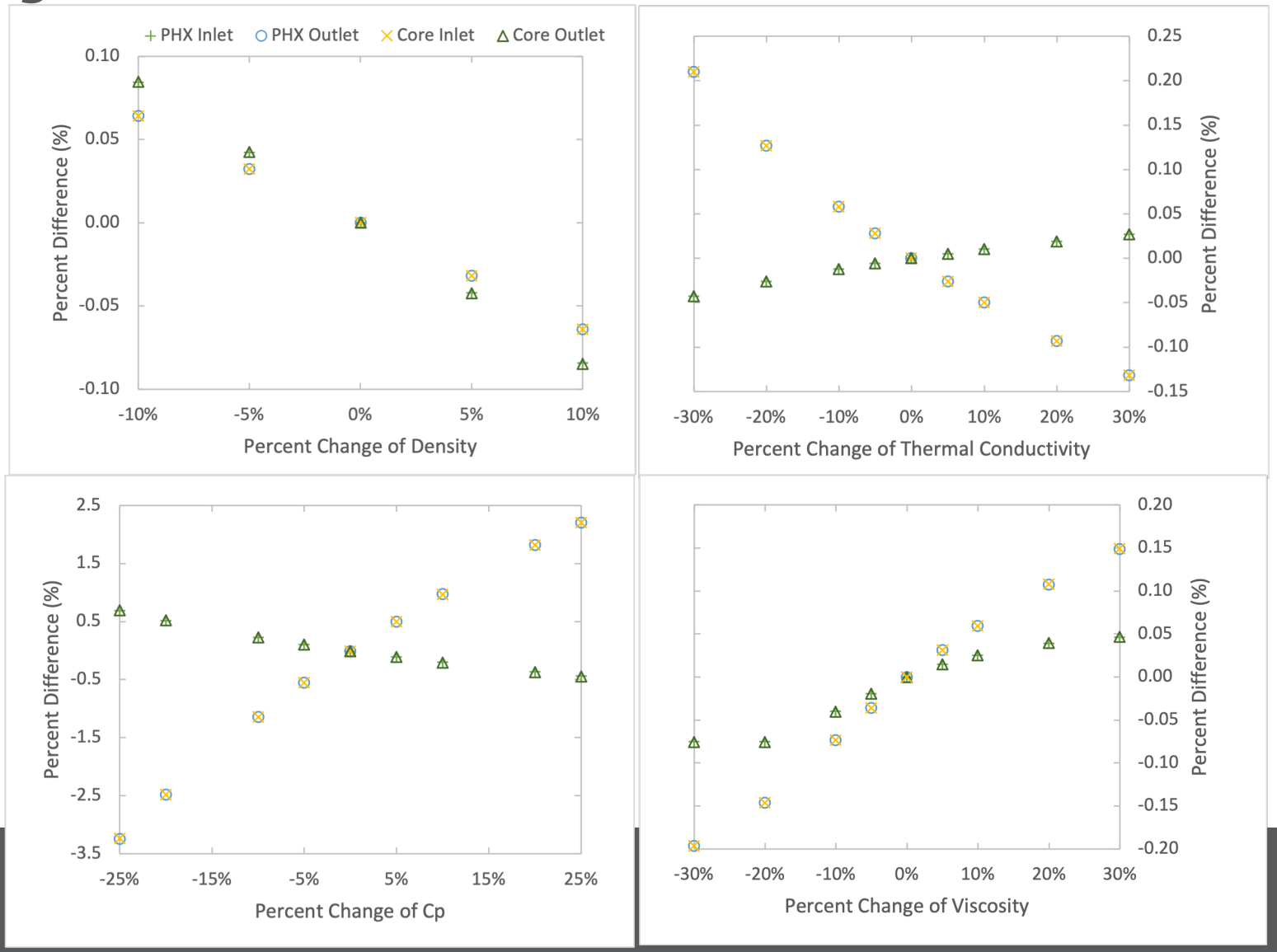








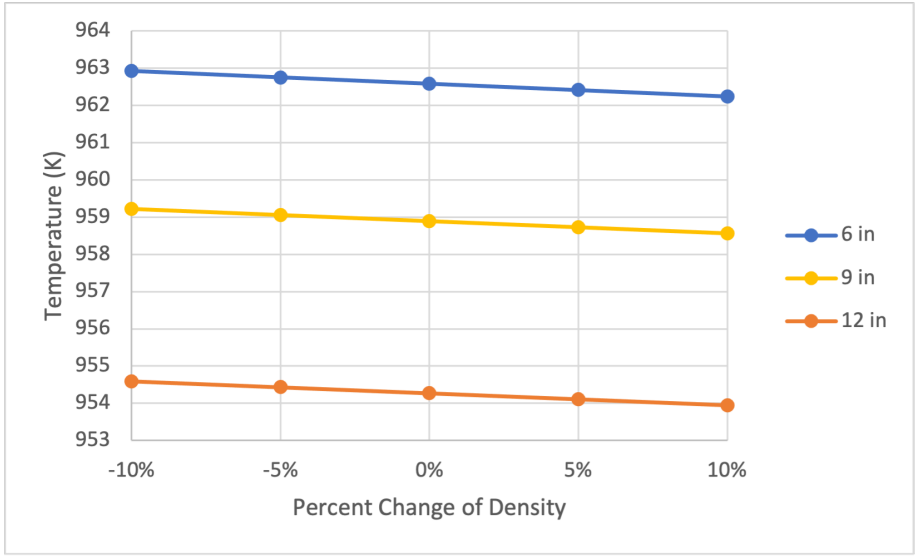
Reactivity Insertion Results

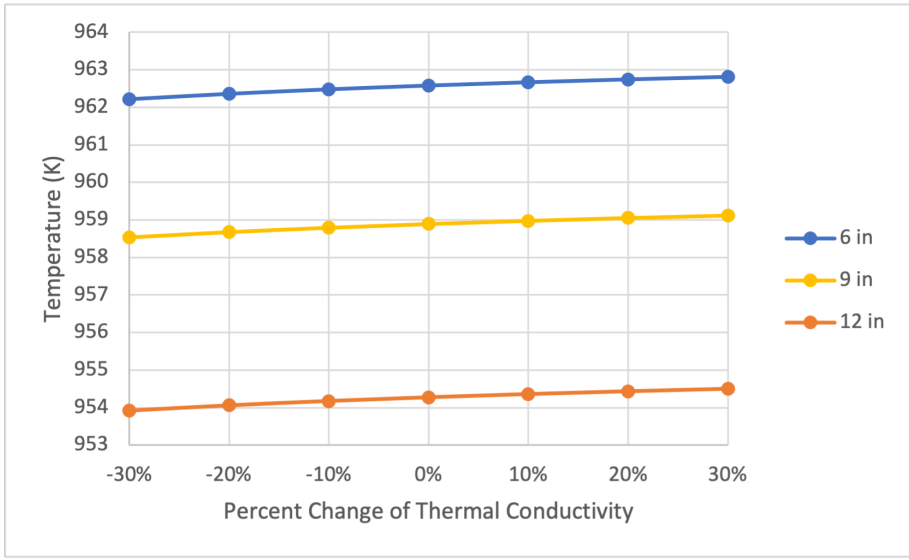


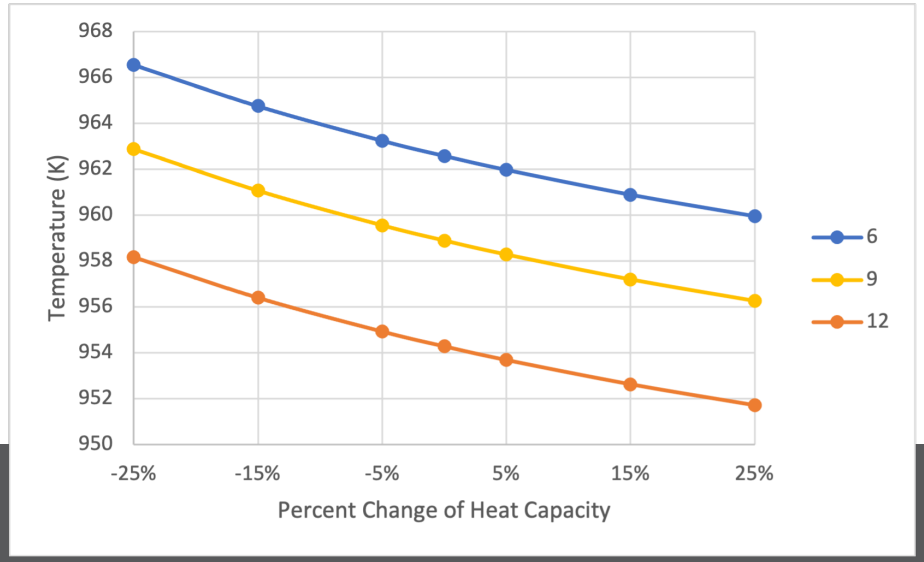
Results

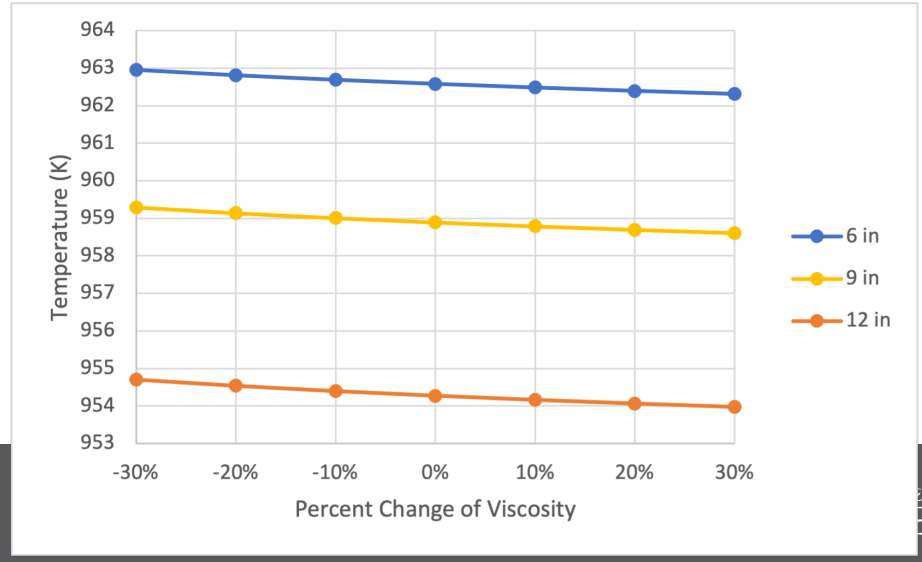
- Steady State
- Reactivity Insertion
- Buildup
  - Plots of property perturbations
- Varying Two Properties at a Time

Buildup Results





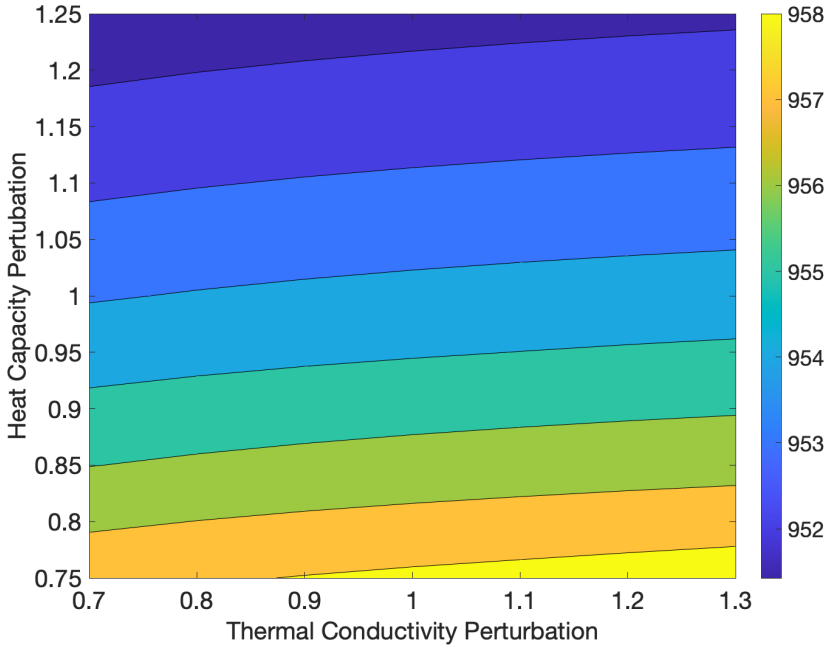


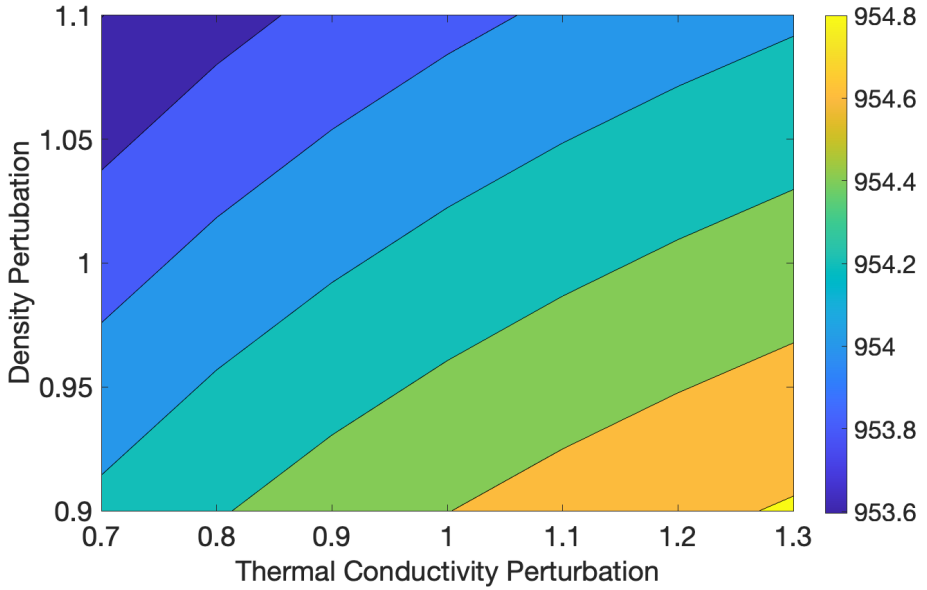


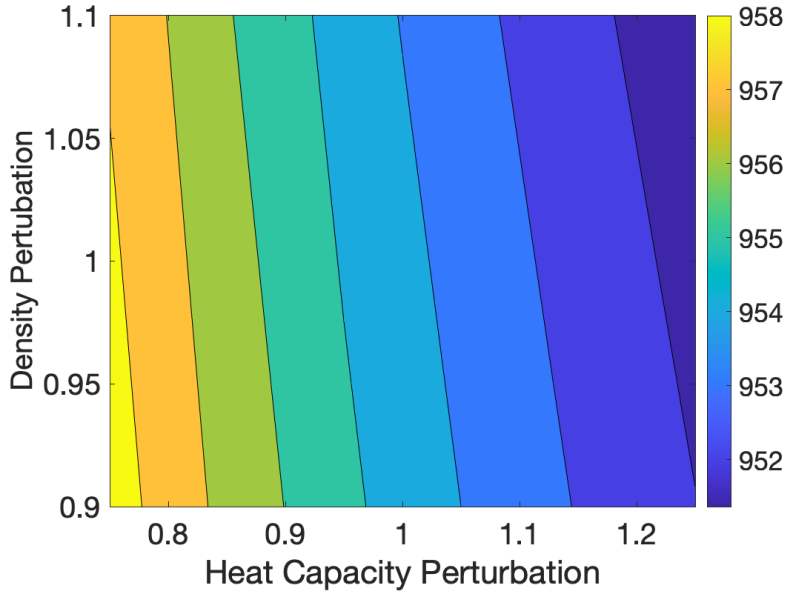
Results

- Steady State
- Reactivity Insertion
- Buildup
- Varying Two Properties at a Time
  - Contour Plots
  - Largest temperature for all perturbations

Two at a Time Results







Results

- Steady State
- Reactivity Insertion
- Buildup
- Varying Two Properties at a Time
  - Contour plots
  - Largest temperature for all perturbations

Two at a Time Results

Property	Largest Temperature (K)	Perturbation Value
Density	954.6	-10%
Thermal Conductivity	954.5	+30%
Heat Capacity	958.2	-25%
Density and Thermal Conductivity	954.8	-10%/+30%
Density and Heat Capacity	958.5	-10%/-25%
Heat Capacity and Thermal Conductivity	958.5	-25%/+30%

Conclusions

- Varying heat capacity had the most affect on the temperature by a wide margin
- Changes in temperature seen, but will not affect safe operation
- Current uncertainty of the four thermophysical properties are well within the bounds of safe operation
- Measurement techniques are adequate

Acknowledgements

- This work was funded by the US DOE Department of Nuclear Energy Advanced Reactor Technology Program.