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Molten Salt Reactor PROGRAM

Update on the Molten Salt Thermal Properties Database-Thermochemical

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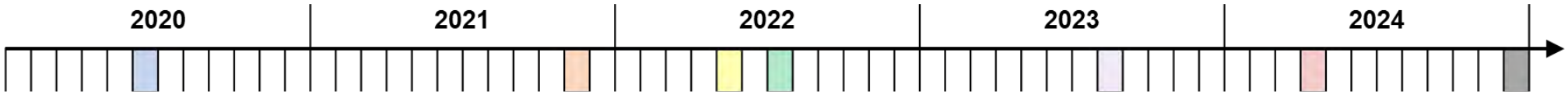
Evolution of MSTDB-TC



MSTDB-TC v.1
Fluorides:
- 48 pseudobinaries
- 28 pseudoternaries

Chlorides
- 12 pseudobinaries
- 1 pseudoternary

Important systems:
- UF_3-UF_4
- LiF-BeF_2-UF_4
- LiF-NaF-KF
- NaCl-UCl_3

Total = 89 systems

MSTDB-TC v.1.2
Fluorides:
- 50 pseudobinaries
- 28 pseudoternaries
- 3 high-order

Chlorides
- 43 pseudobinaries
- 6 pseudoternary
- 2 high-order

Total = 132 systems

MSTDB-TC v.1.3
Fluorides:
- 49 pseudobinaries
- 24 pseudoternaries

Chlorides
- 45 pseudobinaries
- 11 pseudoternaries

MSTDB-TC v.2.0
Fluorides:
- 53 pseudobinaries
- 25 pseudoternaries
- 2 high-order

Chlorides
- 60 pseudobinaries
- 22 pseudoternary
- 3 high-order

Iodides
- 8 pseudobinaries

Major improvements:
- BeF_2 multiple CN
- UF_4 multiple CN
- UCl_3 multiple CN
- Reciprocal systems

Total = 173 systems

MSTDB-TC v.3.0
Fluorides:
- 68 pseudobinaries
- 18 pseudoternaries
- 2 high-order

Chlorides
- 69 pseudobinaries
- 25 pseudoternary
- 3 high-order

Iodides
- 31 pseudobinaries
- 23 pseudoternaries
- 20 high-order

Major improvements:
- Excess C_p
- ZrF_4 systems
- Gas phase
- Corrosion & fission

MSTDB-TC v.3.1 – final touches
Major improvements:
- Noble metal alloys
- Noble gases
- Additional FP
- LiF-NaF-UF_4 fuel
- NaF-KF-UF_4 fuel
- New NaCl-CsCl

MSTDB-TC v.4 – planned
Major improvements:
- $ZrCl_4$ systems
- More RE systems
- Initial oxygen
- Revise FLiBe-CsF,I

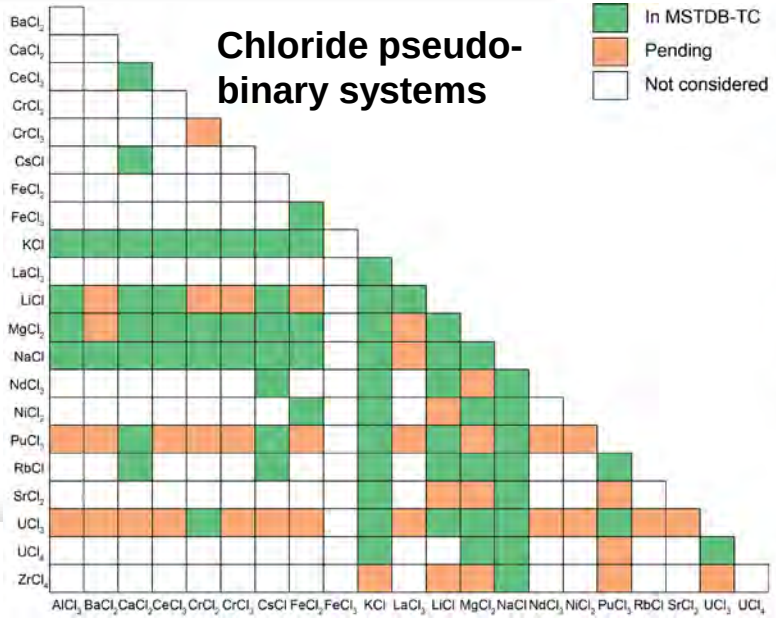
MSTDB-TC Content Now of Sufficient Magnitude to Allow Representing Realistic MSR Systems

	Fluorides	Chlorides	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 cations	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	70 systems	70 systems	30 systems
Pseudo-ternary	30 systems	27 systems	15 systems
Higher order	16 systems	2 systems	All 18 include iodides

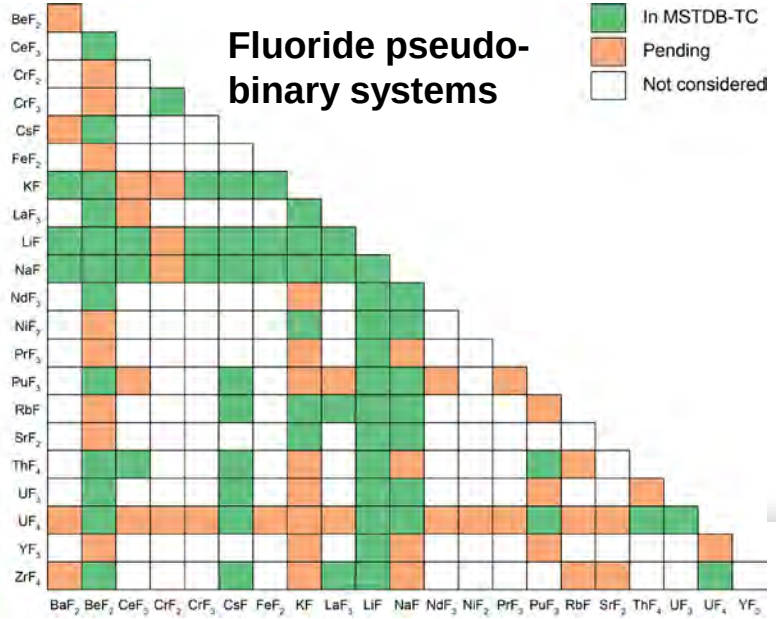
Higher Order Systems

- LiF-LiI-CsI
- LiF-LiI-NaI
- LiF-LiI-KI
- LiF-CsF-CsI
- LiF-KF-KI
- LiF-NaF-NaI
- LiF-NaF-NaI
- NaI-NaF-KF
- KF-KI-NaF
- NaF-NaI-KF
- LiF-NaF-CsI
- LiF-KF-CsI
- LiF-KF-CsI
- NaF-KF-CsI
- LiF-KF-CsF-CsI
- CsI-LiF-NaF-KF
- $MgCl_2$-NaCl-$UCl_{3,4}$
- $MgCl_2$-KCl-$UCl_{3,4}$

Chloride pseudo-binary systems



Fluoride pseudo-binary systems

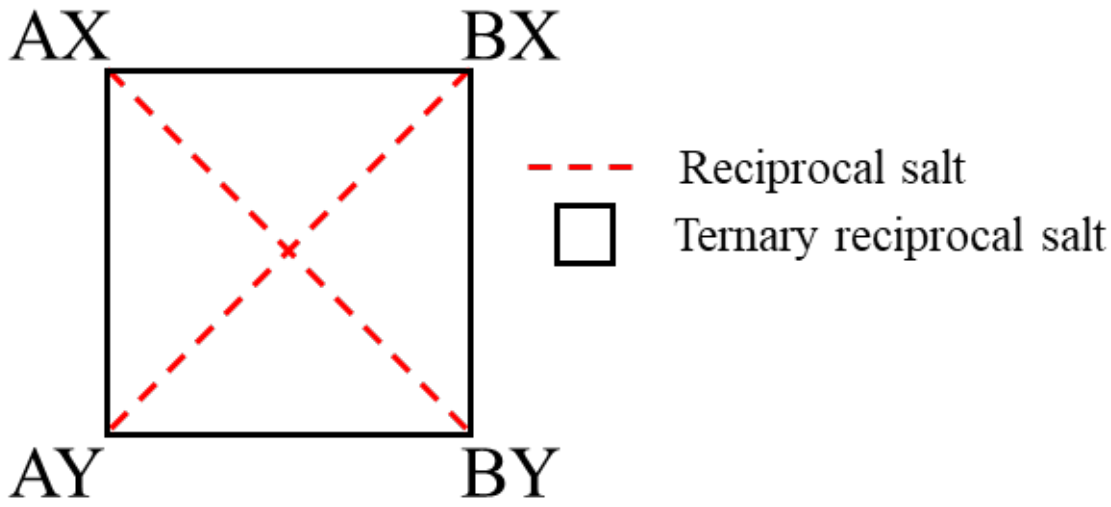


MSTDB-TC Ver. 3.1 Content

Expanded/revised content

- Large increase in reciprocal chloride and fluoride salts with iodine
- Added LiF-NaF-UF_4 and KF-NaF-UF_4 systems
- Revised LiF-NaF-(LaF3, CeF_3, PuF_3) pseudo-ternary systems
- Incorporation of Mo, Ru, Rh, Tc, and Pd alloy and intermetallics based on Kaye et al.*
- Inclusion of He, Ne, Ar, Kr, and Xe, although absent any models for solubility in salts

Reciprocal system of the hypothetical A-B|X-Y species



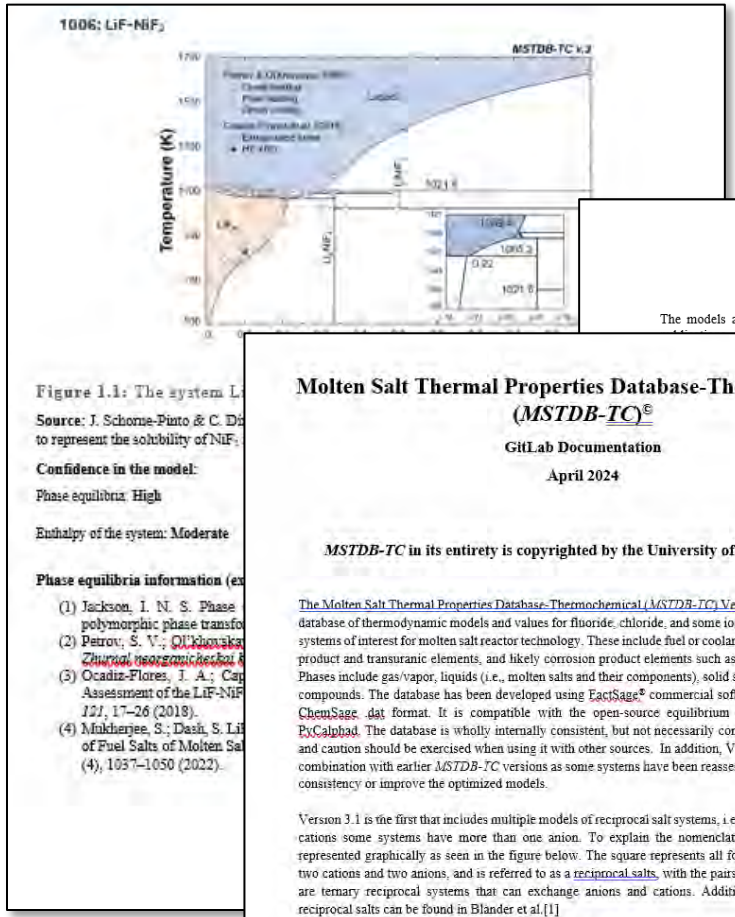
***Thermodynamic Treatment of Noble Metal Fission Products in Nuclear Fuel*."**
Kaye, M.H., B.J. Lewis, and W.T. Thompson, *J. Nucl. Mater.* 366, 1–2 (2007): 8–27

MSTDB-TC Ver. 3.1 Documentation

- Expanded list of references
- Addition internal reports to available references
- Individual 1-2 page descriptions and source information for MSTDB-TC systems not yet in publications
- Expanded “Notes” with key information on usage of MSTDB-TC

Fluorides

- BaF_2-KF [12]
- BaF_2-LiF [1001]
- BaF_2-NaF [12]
- BeF_2-BeI_2 [5]
- BeF_2-CeF_3 [IE]
- BeF_2-CsF [IE]
- BeF_2-LiF [1000]
- BeF_2-LaF_3 [IE]
- CrF_3-KF [23]
- CrF_3-LiF [1004]
- CrF_3-NaF [23]
- CsF-CsI [4602]
- CsF-KF [1]
- CsF-LiF [1]
- CsF-NaF [1]
- CsF-PuF_3 [1009]
- KF-NaF [9]
- KF-NiF_2 [21]
- KF-RbF [17]
- KF-SrF_2 [22]
- KF-UF_4 [17]
- LaF_3-LiF [1400]
- LaF_3-NaF [1403]
- LaF_3-RbF [18]
- LiF-UF_4 [IE]
- LiF-YF_3 [1002]
- LiF-ZrF_4 [1003]
- NaF-NaI [4600]
- NaF-NdF_3 [1407]
- NaF-NiF_2 [21]
- NaF-PuF_3 [1405]
- NaF-RbF [18]


1006: LiF-NiF_2

MSTDB-TC v.3

Temperature (K)

Figure 1.1: The system L

Source: J. Schorne-Pinto & C. Di
to represent the solubility of NiF_2

Confidence in the model:

Phase equilibria: High

Enthalpy of the system: Moderate

Phase equilibria information (ex

(1) Jackson, I. N. S. Phase
polymorphic phase transfo
(2) Petrov, S. V.; Ol'khovska
Zhurnal neorganicheskoi
(3) Ocadiz-Flores, J. A.; Ca
Assessment of the LiF-NiF
121, 17–26 (2018).
(4) Mukherjee, S.; Dash, S. Li
of Fuel Salts of Molten Sa
(4), 1037–1050 (2022).

Notes on Use of *MSTDB-TC*

The models and values provided within *MSTDB-TC* were either directly used as reported in
type system optimizations based on literature-
and new experimental measurements. A system
t experimental and theoretical data are available
and interaction parameters for each phase and
assessed when models and values appropriately
grams) and attendant values such as enthalpy of

base components (i.e., endmembers) in system
om an equilibrium calculation for a mixture may
nt terms may not have been utilized in the system
values for higher order systems caution should
eir accuracy available from the accompanying
acity values for melt solutions are best obtained
e-Thermophysical (*MSTDB-TP*).

d in *MSTDB-TC* should be applied with some
lculations under all conditions can be claimed to
ided below.

contains solution models that incorporate many
tions to be performed in codes such as FactSage
n the database. That means that calculations can
or eight or more cations in the melt even though
ee cations that have been optimized (see the list
B-TC documentation). Thus, the results of such
not be claimed as having been performed using
caution in claiming the validity of results for
ed, in reality, these should be relatively accurate
action parameters in salt melt models beyond the
al reality which makes unlikely simultaneous
s in the melt.)

only a constrained composition region as either
hat region, or it was not possible to reasonably fit
using the current modeling frameworks or single
he case, efforts were made to best represent
value for molten salt reactor applications. That
roduction of low concentration regions for fission
oid computing equilibria for compositions which
the table below that identifies issues with some

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

GitLab Documentation

April 2024

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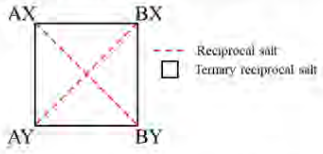
The Molten Salt Thermal Properties Database-Thermochemical (*MSTDB-TC*) Ver. 3.1, is a publicly available database of thermodynamic models and values for fluoride, chloride, and some iodide components and related systems of interest for molten salt reactor technology. These include fuel or coolant salts, consequential fission product and transuranic elements, and likely corrosion product elements such as iron, nickel and chromium. Phases include gas/vapor, liquids (i.e., molten salts and their components), solid solutions, and stoichiometric compounds. The database has been developed using FactSage® commercial software and is provided in the ChemSage .dat format. It is compatible with the open-source equilibrium codes Thermochimica and PyCalphad. The database is wholly internally consistent, but not necessarily consistent with other databases and caution should be exercised when using it with other sources. In addition, Ver. 3.1 should not be used in combination with earlier *MSTDB-TC* versions as some systems have been reassessed for Ver. 3.1 to maintain consistency or improve the optimized models.

Version 3.1 is the first that includes multiple models of reciprocal salt systems, i.e., that in addition to multiple cations some systems have more than one anion. To explain the nomenclature, reciprocal systems are represented graphically as seen in the figure below. The square represents all four species of a system with two cations and two anions, and is referred to as a reciprocal salts, with the pairs connected by the diagonals are ternary reciprocal systems that can exchange anions and cations. Additional information regarding reciprocal salts can be found in Blander et al.[1]



Reciprocal system of the hypothetical A-B|X-Y species

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Questions

Your email Address

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