Molten Salt Thermodynamic Database-Thermochemical (*MSTDB-TC*)

GitLab Documentation

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Use the following references when citing *MSDTB-TC*

J.C. Ard, J.A. Yingling, K.E. Johnson, J. Schorne-Pinto, M. Aziziha, C.M. Dixon, et al. *Development of the Molten Salt Thermal Properties Database − Thermochemical (MSTDB−TC), example applications, and LiCl−RbCl and UF_3−UF_4 system assessments.* J. Nucl. Mat. 2022. 563: 153631. https://doi.org/10.1016/j.jnucmat.2022.153631.

Developing Practical Models of Complex Salts for Molten Salt Reactors. Besmann, T.M. Schorne-Pinto, J., Thermo, 1 168–178 (2021). https://doi.org/10.3390/thermo1020012

1. Introduction

The Molten Salt Thermal Properties Database-Thermochemical (*MSTDB-TC*) is 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 iron, nickel and chromium. Phases include gas/vapor, liquids (e.g., molten salts, noble metals), and solid compounds. Solutions include the fluoride-based and chloride-based liquid melts as well as several solid solutions. The database was developed in the ChemSage .dat format using the FactSage® commercial package and compatible with the open-source equilibrium code Thermochimica.

The models and values provided within *MSTDB-TC* are obtained through combinations of literature-reported information, first principles calculations, and experimental measurements. These have been used to a greater or lesser extent as needed in assessments for pseudo-binary, pseudo-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 to represent each phase in that system. In essence, a system is assessed when models and values appropriately reproduce available phase equilibria (phase diagram) and attendant values such as heat capacity, enthalpy of mixing, and vapor pressures.

Maintaining consistency of pure compound thermodynamic values throughout the database is vital. Pure compound values provide the foundation from which solutions are modeled. As each compound in the solution can be a part of multiple different subsystems, the underlying pure compound values need to be the same across all solutions. In order to accomplish this, a single set of thermodynamic values need to be selected for each compound, which is used for all subsequent solutions. An effort has been made to select the best available thermodynamic values for pure compounds, as any need to change the values in the future may require a substantial re-assessment effort of all affected systems. Due to differences in pure compound values between different publications and those selected for the *MSTDB-TC*, it often became necessary to perform re-assessments of published solution models before being added to the database. If the pure compound values did not differ greatly, the re-assessment could be slight, or even unnecessary.

A note of caution: It is possible to perform thermodynamic equilibrium calculation with FactSage. Thermochimica, or other software using *MSTDB-TC* for salt melts that contain multiple cations. While the calculations may run smoothly, the results might not be accurate as the specific combination of the salt cations for the halide melt may not have been assessed and therefore known to reproduce observed behavior. The user is advised to check the listing of *MSTDB-TC* systems to be assured that their system of interest has been included.

2. Database Contents

The *MSTDB-TC* has been prepared for public release through the code.ornl GitLab repository hosted by Oak Ridge National Laboratory. The repository includes the following files for the latest version of the *MSTDB-TC*:

- The database .dat files in standard ChemSage ASCII format, which contain all compounds and solutions of the *MSTDB-TC* for the fluoride- and chloride-based systems, respectively (denoted by Fluorides or Chlorides in .dat file name). Separate sets of .dat files provided for compatibility with different software and versions:
    - FactSage 8.1 compatible .dat files end in *_8-1.dat
        - Generated in FactSage 8.1 with “include functions” selected.

    - FactSage 8.0 (and earlier) as well as most other software compatible .dat files end in *_8-0.dat
        - Generated in FactSage 8.1 with “include functions” not selected.
- Documentation Excel files (data packages) provided for each subsystem, which are intended to make information easily traceable to original sources. The data packages provide an account of all pure compounds, liquid solutions and solid solutions used in modeling the subsystem with linked references. Modeling parameters from newly performed work are also reported in the data package along with any applicable references.
- An Excel file containing the thermodynamic values used for all pure compounds of the *MSTDB* along with linked references.
- A pair of pdfs of all modeled pseudo-binary and pseudo-ternary phase diagrams for the fluoride- and chloride-based systems, respectively (denoted by Fluorides or Chlorides in pdf file name). Calculated diagrams in pdf are calculated using the current *MSTDB-TC* version alongside available published phase diagrams (with references). Used as part of internal Quality Assurance (QA) effort.
- Readme files in the code.ornl readable format for each of the major directories of the repository. These files provide details and explanation of the files contained within each major directory.

The remaining sections list the modeled systems and solid solutions within the *MSTDB-TC*.

2.1 Pseudo-binary Systems

Fluorides

- BeF_2-KF
- BeF_2-LiF
- BeF_2-NaF
- BeF_2-PuF_3
- BeF_2-ThF_4
- BeF_2-UF_4
- CaF_2-BeF_2
- 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-KF
- CsF-LiF
- CsF-NaF
- CsF-RbF
- CsF-ThF_4
- CsF-UF_3
- 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-NaF
- LiF-NdF_3
- LiF-NiF_2
- LiF-PuF_3
- LiF-RbF
- LiF-ThF_4
- LiF-UF_3
- LiF-UF_4
- 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
- $CrCl_2$-NaCl
- 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
- KCl-LiCl
- KCl-$MgCl_2$
- KCl-NaCl
- KCl-$NiCl_2$
- KCl-RbCl
- KCl-UCl_3
- K-KCl
- LiCl-$MgCl_2$
- LiCl-NaCl
- LiCl-RbCl
- LiCl-UCl_3
- $MgCl_2$-NaCl
- $MgCl_2$-$NiCl_2$
- $MgCl_2$-RbCl
- Mg-$MgCl_2$
- NaCl-$NiCl_2$
- NaCl-RbCl
- NaCl-UCl_3
- $PuCl_3$-RbCl

2.2 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-NaF-UF_4
- 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
- CsF-KF-LiF
- 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-$MgCl_2$
- LiCl-KCl-UCl_3

2.3 Solid Solutions

Fluorides

- SSaa = $(Li, Na)_7Th_6F_{31}$
- SSab = $(Pu, Th)F_x$
- SSac = $Li(Th, U)_4F_{17}$
- SSad = $Li(Th, U)_2F_9$
- SSae = $Li_7(Th, U)_6F_{31}$
- SSaf = $Li_3(Th, U)F_7$
- SSag = $Na_2(Th, U)F_6$
- SSah = $Na_7(Th, U)_6F_{31}$
- SSai = $Na(Th, U)_2F_9$
- SSam = (Li, Na, K, Rb, Cs)F
- SSan = $(Ce, Th)F_x$
- SSao = $(Ca, Th)F_x$
- SSap = $(Ca, La)F_x$ (LaF_3 destabilized)
- SSaq = $(Ca, La)F_x$ (CaF_2 destabilized)
- SSar = $(La, Pu)F_x$
- SSas = $(Na, Th)F_x$
- SSat = $(U, Pu)F_x$
- SSau = $(U, Th)F_x$
- SSav = Li_3ThF_7-BeF_2-LiBeThF$_7$
- SSaw = $(Li, Na)_7U_6F_{31}$
- SSax = $Na_7(Th, U)_2F_{15}$
- SSay = $Na_3Th_2F_{11}$-$Na_5U_3F_{17}$
- SSaz = $(Li,Ni)F_x$
- SSba = $Na_5Nd_9F_{32}$-NaF
- SSbb = $(Na,Ce)F_x$
- UF34 = $UF_{(3+x)}$

Chlorides

- SScb = (Li,K)Cl
- SScc = (Li,K)Cl
- SSce = $(Li,Mg)Cl_x$
- SScf = $(Li,Mg)Cl_x$
- SScg = $(Na,K)_2CeCl_5$
- SSch = $(Na,K)_3CeCl_6$
- SSci = $(Na,K)_3Ce_5Cl_{18}$
- SScj = $(Fe,Mg)Cl_2$
- SSck = $(Mg,Ni)Cl_2$
- SScl = $(Mg,Ni)Cl_2$
- SScm = $(Fe,Ni)Cl_2$
- SScn = $(Fe,Ni)Cl_2$
- SSco = (Li,Na)Cl
- SScq = $(Na,Ca)Cl_x$
- SScr = $(Mg,Ca)Cl_2$
- SScs = (Na,K,Rb,Cs)Cl

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Ref. Number	Authors	Year	Title	Publication	Issue/Chapter	Pages	ORNL Doc #
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2	O. Benes, R.J.M Konings	2008	Thermodynamic evaluation of the MF-LaF3 (M = Li, Na, K, Rb, Cs) systems	Calphad-Computer Coupling of Phase Diagrams and Thermochemistry	32	121-128	
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