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An Overview of the Molten Salt Thermal Properties Database–Thermophysical, Version 3.1 (MSTDB-TP v.3.1)

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September 2024

OAK RIDGE National Laboratory

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US Department of Energy–Office of Nuclear Energy, Nuclear Energy Advanced Modeling and Simulation Program

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ABBREVIATIONS

AIMD	*ab initio* molecular dynamics
Argonne	Argonne National Laboratory
CAC	common access card
CI/CD	continuous integration and continuous delivery
CSV	comma separated value
DOE-NE	Department of Energy, Office of Nuclear Energy
DOI	digital object identifier
ITSD	Information Technology Services Division
MSR	molten salt reactor
MSTDB	Molten Salt Thermal Properties Database
MSTDB-TC	Molten Salt Thermal Properties Database – Thermochemical
MSTDB-TP	Molten Salt Thermal Properties Database – Thermophysical
NEAMS	Nuclear Energy Advanced Modeling and Simulation
ORNL	Oak Ridge National Laboratory
RK	Redlich–Kister

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ABSTRACT

This report presents the current status of the Molten Salt Thermal Properties Database–Thermophysical (MSTDB-TP). Information regarding version 3.1 is provided herein, which contains 820 individual salt entries (data from 180+ independent studies); the thermophysical properties contained in the database include density, viscosity, thermal conductivity, and heat capacity. The major updates to the database include a significant expansion of pseudobinary and higher-order chloride salt mixtures, many of which bearing actinides, and an incorporation of more recent literature data (i.e., that within the past 5 years). Also, modifications have been made to the pure compound data in the database as a consequence of an external quality assessment of duplicate datasets. The user-facing API for the MSTDB-TP, Saline, has been updated to include viscosity estimation capabilities based on the Redlich–Kister formalism; this is an advancement with respect to the existing density estimation capabilities. The graphical user interface was also updated to include a density estimation capability, backed by Saline. Finally, additional preliminary efforts to include surface tension into the database, as well as an investigation on formalisms that would be appropriate for thermal conductivity estimation, are reported herein.

1. INTRODUCTION

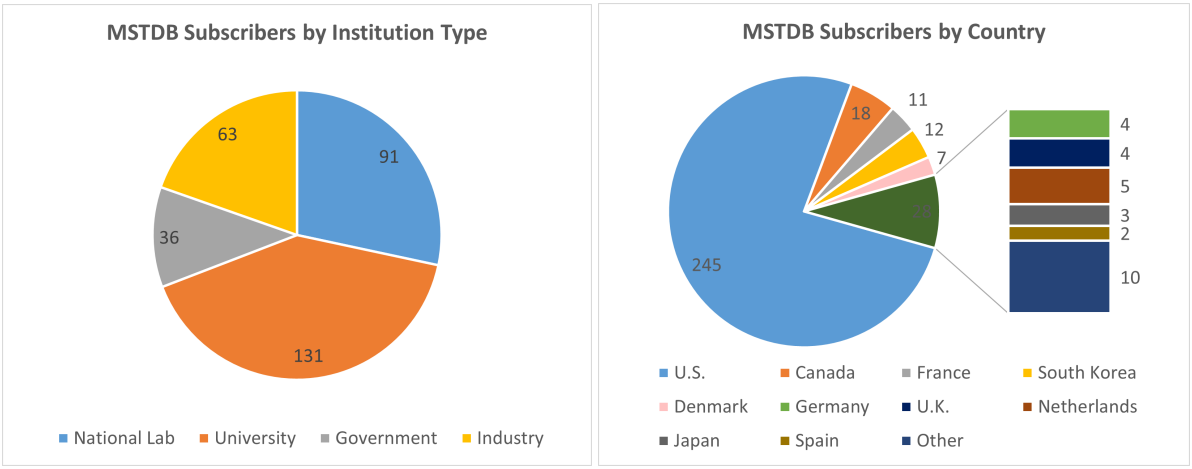
The Molten Salt Thermal Properties Database (MSTDB) is a US Department of Energy, Office of Nuclear Energy (DOE-NE) funded database that includes thermal properties of a wide array of molten salt compounds and multi-component systems that are candidate materials for molten salt reactor (MSR) coolants and fuels. The database contains two arms, the thermophysical arm (TP) and the thermochemical arm (TC). MSTDB-TP contains correlations that describe thermophysical properties as a function of temperature, for key compounds and mixtures, whereas MSTDB-TC contains thermodynamic models based on Gibbs energy relations. Both arms and associated documents are hosted on a publicly accessible, permission-protected server at Oak Ridge National Laboratory (ORNL). This report focuses on the current version of MSTDB-TP, but more information regarding MSTDB-TC can be found on the MSTDB website and in peer-reviewed publications regarding MSTDB-TC and its applications [2, 3].

The motivation behind the MSTDB-TP is to support thermal hydraulic and multiphysics simulation of MSRs. The chloride and fluoride compounds and multi-component systems of interest for the MSR developers have been outlined in a roadmap for thermal property measurements published in 2021 [4]. The roadmap has allowed for the formation of a matrix of pseudobinary systems, comprising key molten salt compounds for coolants and fuel that may serve as systems or subsystems of interest for reactors currently under development. Because several designs are currently under development with different fuel and coolant compositions [5, 6, 7, 8, 9], it is important to, as exhaustively as possible, fill the existing gaps within this matrix based on experimental and simulated data. Furthermore, the data selected and put into the primary database file—which represents the suggested references for specific molten salt systems by the MSTDB-TP developers—should be the most accurate data to the developers' knowledge; this way, the MSR design process will not be ill-informed from a thermophysical property standpoint. Therefore, MSTDB-TP developers, in collaboration with external partners, have carefully selected single datasets out of duplicate datasets and have chosen to exclude certain datasets for which there exist unique measurements (for example, some higher-order actinide–bearing fluoride thermal conductivity measurements), due to particularly poor experimental controls and highly questionable data.

The MSTDB-TP effort, funded by the DOE-NE Nuclear Energy Advanced Modeling and Simulation (NEAMS) program, has good synergy with the DOE-NE MSR Program. Under the MSR program, several national laboratories are performing thermophysical property measurements that can be incorporated into the MSTDB-TP [10, 11, 12, 13, 14]. This way, the database's existing data can be better validated (as some of the data are over five decades old), and some of the gaps can be filled, thereby improving the overall understanding of how thermophysical properties change as a function of the compositional space of the chloride and fluoride matrices. Furthermore, molecular dynamics studies, which are funded under both the MSR and NEAMS programs [15, 16], can provide thermophysical property predictions as well as key insights into why properties may exhibit certain non-ideal trends due to changes in coordination chemistry and ion mobility. Finally, external review of the data in the database is being conducted to assess the quality of the experimental studies that have been conducted to collect the thermophysical property data, and this effort is allowing for more careful selection of properties going forward.

MSTDB-TP has a variety of user types. Currently, there are a total of 321 users, and the distribution of users is shown in Fig. 1. Among these users, it is anticipated that some fraction (namely among the national laboratory users) is using MSTDB-TP in high-fidelity simulations of multiphysics, thermal hydraulics, neutronics, or species tracking. These users benefit from a robust, high-speed interface with the MSTDB-TP to rapidly extract thermophysical property values of need. The user base also includes

experimentalists and molecular dynamics modelers, who generally need limited information from the database and generally seek validation data to compare against their experiments/models. Finally, private entities may need the MSTDB-TP data for a variety of use cases, including those mentioned already, and also for design licensing purposes. Given the variety of user types and use cases, MSTDB-TP has both an API called Saline and a graphical user interface (GUI), which have both been reported previously [17, 18], and updates to these tools are provided herein.



(a) (b)

Figure 1. Breakdown of MSTDB subscribers. (a) A breakdown by institution type and (b) a breakdown by country.

The number of gaps that exist in the database will be difficult to fully experimentally quantify—or even quantify with accurate molecular dynamics studies, such as *ab initio* molecular dynamics (AIMD), within a desirable time frame given the different MSR developers' timelines for deployment. Therefore, rapid estimation tools that leverage MSTDB-TP are desirable to flesh out the gaps in the MSTDB-TP pseudobinary matrix, as well as to provide a capability to extrapolate data to arbitrarily sized, higher-order systems. A Redlich–Kister (RK) based formalism has been employed in the MSTDB-TP to enable such predictions. Of course, such an implementation is not meant to replace the need for experimental measurements for the quantification of molten salt systems of interest to MSR developers; rather, RK models were employed in MSTDB-TP to enable scoping studies, inform thermal hydraulic performance with a moderate level of uncertainty, and allow researchers to better understand general trends in the compositional and temperature dependence of the thermophysical properties.

2. DATABASE COMPOSITION

Currently, the TP data held in MSTDB-TP consist of compiled data from more than 180 published studies conducted by various laboratories, industries, and university projects. The data held in the ORNL GitLab server consists of two CSV files: one containing all the property data for each salt and their respective compositions and the other containing reference data (full references and DOIs). The property data for molten salts include the following:

- Melting temperature

- Boiling temperature
- Density
- Viscosity
- Thermal conductivity
- Heat capacity

For each property, a shorthand reference, experimentally measured range, empirical constants, and an estimation of the measurement errors are provided. Although all properties are present in the database, each entry (i.e., one specific salt mixture) may not contain all the properties. Property availability for salt mixtures with up to four components are shown in Figures 2 and 3. Each table or figure shows the salt property data available in the database, as well as the number of measurements over each salt's compositional space that have been recorded for each property.

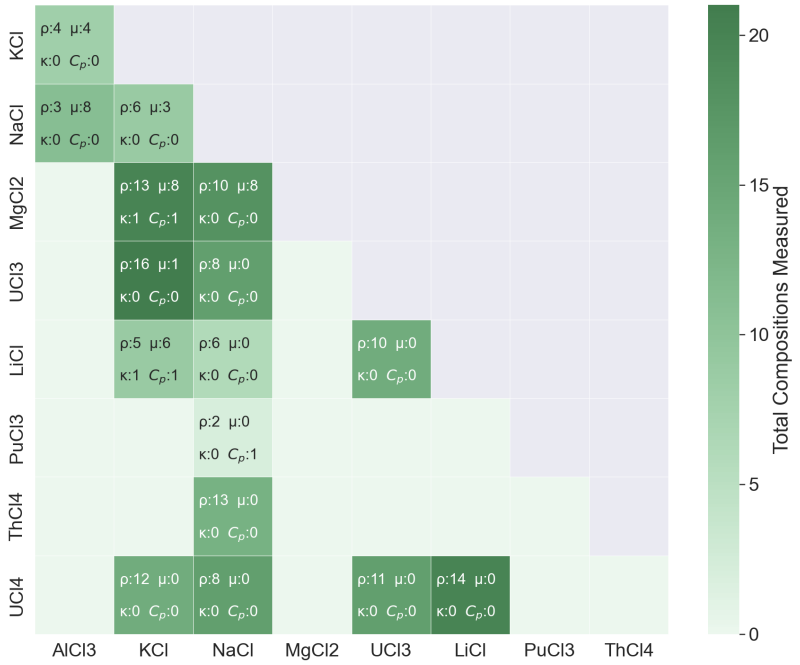
In addition to these two CSV files, two CSV files containing RK parameters for density and viscosity estimation for select pseudobinary mixtures in MSTDB-TP are also stored on the GitLab server; more details on these files are provided in Section 2.3.

Notably, MSTDB-TP and MSTDB-TC are consistent regarding multicomponent system melting points and pure compound heat capacities. All multicomponent salt systems that have been thermodynamically evaluated by MSTDB-TC v3.1 have had their melting points calculated for MSTDB-TP by the Thermochimica software using the Gibbs energy models in the MSTDB-TC database. Those systems that have not been evaluated by MSTDB-TC 3.1 use existing experimental melting point literature data for reporting in MSTDB-TP, if available. Heat capacity values for pure compounds have been extracted from the thermodynamic value tabulations within MSTDB-TC, and source references have been associated when available. Notably, multicomponent system heat capacities in MSTDB-TP do not mimic MSTDB-TC model outputs; rather, they are extracted directly from experimental values in the literature.

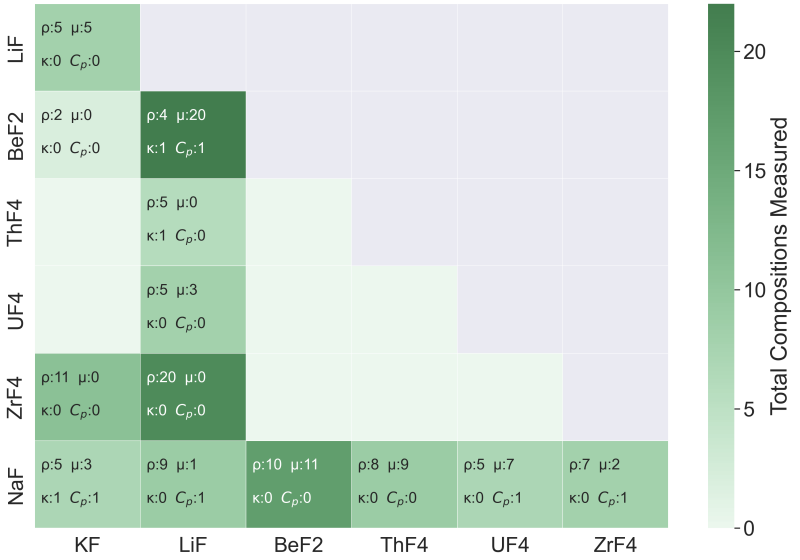
2.1 ADDITIONS FROM 3.0 UPDATE

The primary change between MSTDB-TP 2.1 [18] and MSTDB-TP 3.0 was the inclusion of a significant quantity of pseudobinary and pseudoternary chloride system data, including UCl_3 and UCl_4. This also includes viscosity data for the UCl_3 and UCl_4 endmembers that were previously not known, enabling formation of RK models of these properties. Previously, the pseudobinary and pseudoternary data were significantly lacking for chloride systems, and this update provides significantly more data to generally inform fast reactor development, while the significant quantity of data on fluoride systems already in the database generally supports thermal reactor development.

The inclusion of such a large quantity of chlorides was enabled due to an assessment of a compilation of Russian experimental efforts by Katyshev [19]. Extraction of the data was challenging because the underlying text is in Russian and the quantities are reported as molar properties. After translation, manual extraction, and conversion to standard international units, the properties were then assessed for uncertainty by comparing density and viscosity of alkali chloride endmembers to the existing values in the database for which the uncertainties have already been critically evaluated. Such a comparison allowed for conservative assignment of uncertainty, along with a general understanding of typical uncertainty values associated with the methods used. Additional validation through validating experimentation by the MSR program will



Chloride pseudobinary salts



Fluoride pseudobinary salts

Figure 2. Heat map of measured properties for chloride and fluoride pseudobinary salts in MSTDB-TP v3.1.

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	0	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	0	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	1	0	1
UCl4	1	1	0	0
UF3	0	0	0	1
UF4	1	1	0	1
ZrCl4	1	1	0	0
ZrF4	1	0	0	0

Salt	Measurements			
	ρ	μ	κ	c_p
KCl-LiCl-NaCl	4	0	0	0
KCl-LiCl-UCl3	18	0	0	0
KCl-LiCl-UCl4	18	0	0	0
KCl-NaCl-UCl3	18	0	0	0
KCl-UCl3-UCl4	32	0	0	0
AlCl3-LiCl-NaCl	10	10	0	0
LiCl-UCl3-UCl4	21	0	0	0
BeF2-LiF-ThF4	3	2	0	0
BeF2-LiF-ZrF4	1	0	0	0
BeF2-LiF-NaF	5	4	0	5
KF-LiF-NaF	1	1	1	1
LiF-NaF-ZrF4	11	2	2	2
BeF2-LiF-UF4	36	38	2	0
LiF-ThF4-UF4	1	0	0	0
KCl-MgCl2-NaCl	1	1	1	1
LiCl-NaCl-UCl3	18	0	0	0
LiCl-NaCl-UCl4	18	0	0	0
NaCl-UCl3-UCl4	26	0	0	0
BeF2-NaF-UF4	79	71	0	0
BeF2-KF-NaF	1	1	0	1
KF-MgF2-NaF	1	0	1	1
KF-NaF-UF4	3	1	0	2
KF-NaF-ZrF4	1	1	0	1
NaF-UF4-ZrF4	5	4	0	6
RbF-UF4-ZrF4	2	2	0	2

Salt	Measurements			
	ρ	μ	κ	c_p
BeF2-LiF-ThF4-UF4	1	1	1	1
BeF2-LiF-UF4-ZrF4	1	0	1	0
BeF2-NaF-UF4-ZrF4	1	0	0	0
BeF2-LiF-NaF-UF4	1	1	0	1
KF-LiF-NaF-UF4	2	2	0	2
LiF-NaF-UF4-ZrF4	1	1	0	2
KF-NaF-UF4-ZrF4	0	0	0	2

Figure 3. Tables of the number of measured properties in MSTDB-TP v3.1 for pure, pseudoternary, and pseudoquaternary salts.

allow for these uncertainty assumptions to be better informed; for example, the UCl_3-bearing salt density studies by Parker et al. [10] are particularly useful in this regard.

In addition to the inclusion of the chloride system data from Katyshev, a small quantity of higher-order, actinide-bearing fluoride system data were added, including density and thermal conductivity values. Some thermal conductivity data originally in the database for higher-order, actinide-bearing fluoride systems—originating in Powers [20]—were determined to be unreliable and were removed from the database in the 3.0 update. Although the heat capacity values put forth by Powers seem reasonable based on comparison with critical evaluations of FLiNaK and FLiBe [21, 22], the thermal conductivity measured by Powers for FLiNaK was ~6 times higher than critically evaluated thermal conductivity data for FLiNaK [21], leading to a general lack of trust in the thermal conductivity values of higher-order, actinide-bearing fluoride systems measured by Powers.

Finally, the 3.0 update incorporated some reciprocal salt systems taken from the assessment of Katyshev's compilation; these systems are composed of base compounds of interest to the MSR developers [4]. The expansion of the RK parameters that could be quantified as a consequence of the 3.0 update is outlined in Section 2.3.

2.2 ADDITIONS FROM 3.1 UPDATE

There were two major aspects of the update from MSTDB-TP 3.0 to 3.1. The first major aspect was the modification of pure compound (i.e., endmember) data in the database for fluorides, as a consequence of an external application of quality rankings of duplicate datasets in the literature by our collaborators at Argonne National Laboratory (Argonne) [11, 23]. This affected density dataset selection for BeF_2 and NaF. This also affected viscosity dataset selection for BeF_2, KF and NaF. It should be noted that duplicate data are not stored in the main CSV file for MSTDB-TP; only the datasets considered to be most accurate are put forth as recommended data in this file. The assessments of the duplicate data for fluorides can be found in public reporting by Argonne. The quality rankings are also stored on a currently private project on the ORNL hosted GitLab server, with plans to make all duplicate data and associated quality rankings public when the broad application to MSTDB-TP is finalized. It should be noted that this effort is an ongoing endeavor led by Argonne under the MSR program.

Other additions to 3.1 included the incorporation of more recent literature data—acquired by universities or laboratories in approximately the past 5 years—to ensure that MSTDB-TP includes recent data. A particular focus was to ensure the inclusion of additional thermal conductivity data, given the overall sparseness of data associated with that property. Some of the recent studies were excluded if the measurement approach used therein could not be validated (e.g., via calibration with a well-characterized salt or thorough uncertainty propagation) or if the values appeared particularly erroneous based on an understanding of the endmember properties. Some notable additions include assessed recent data on KF-BeF_2, LiF-NaF-ZrF_4, LiF-BeF_2-UF_4, NaCl-KCl-$MgCl_2$, NaF-KF-MgF_2.

2.3 REDLICH–KISTER EXPANSION AND MUGGIANU INTERPOLATION

RK models have been developed for both density and viscosity for interpolation within the temporal and compositional space for pseudobinary systems, as well as extrapolation to higher-order systems based on pseudobinary subsystems. The mathematical formalisms are derived in previous publications [24, 25, 26], but the overall scheme for the modeling is discussed herein. An example of how the RK model is applied is shown in Fig. 4 for LiCl-KCl. The density model relies on an ideal component that is based on additive

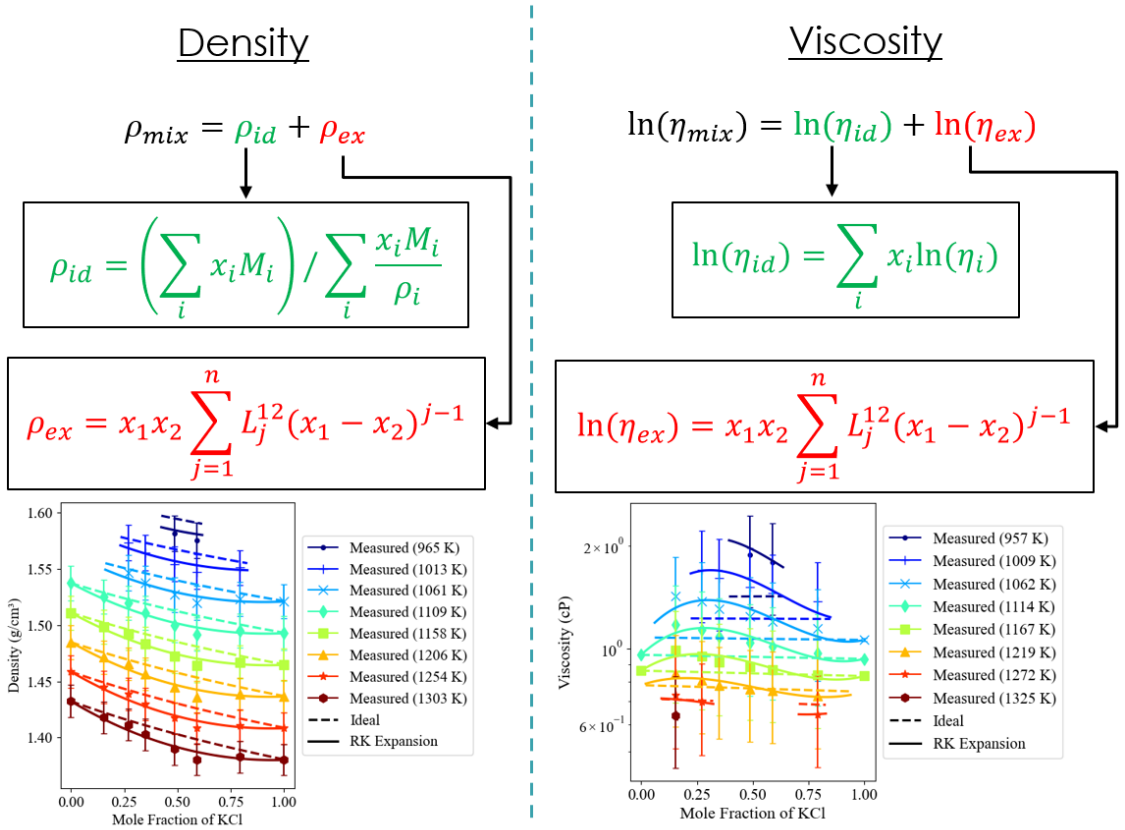


Figure 4. Example of the application of the RK formalism to interpolate density and viscosity in the LiCl-KCl system.

molar volumes, whereas the viscosity model relies on an ideal component based on the Grunburg–Nissan mixing rule. The ideal models for the LiCl-KCl system specifically are quite close to the experimental data because alkali halides that are dissociated in the melt tend to exhibit ideal mixing.

However, the slight non-idealities observed can be quantified by regression of an RK expansion to fit a combination of ideal and non-ideal components in the model to the data. Currently, a non-linear least squares fitting approach is employed, and uncertainties are understood based on the associated covariance matrices [25, 26]. The resultant RK models, which include the non-ideal term, fit to the experimental data to account for the non-ideal mixing behavior. If LiCl-KCl represents a subsystem of a higher-order system, then Muggianu extrapolation is employed to inform the higher-order model, which can be fully described only if all the pseudobinary subsystems have quantified RK parameters. This approach relies on an underlying trust in the experimental data to which the RK model is fit—and thus the continuing work to better identify the most trustworthy data among duplicate datasets, in collaboration with Argonne, is particularly important in ensuring that the non-ideal behavior being modeled is accurately informed.

The total list of RK parameters in the MSTDB-TP, for density and viscosity, is provided in Tables 1 and 2. The temperature-dependent constants in the non-ideal components of the model L_j^{12} are defined by

$$L_j^{12} = A_j^{12} + B_j^{12}T \tag{1}$$

for density and

$$L_j^{12} = A_j^{12} + B_j^{12}T + C_j^{12}T^2 \tag{2}$$

for viscosity.

Table 1. Redlich-Kister parameters in MSTDB-TP v3.1 for density estimation.

Salt 1	Salt 2	A_1^{12} (g/cm^3)	B_1^{12} (g/cm^3T)	A_2^{12} (g/cm^3)	B_2^{12} (g/cm^3T)
KCl	NaCl	-0.03013	-1.210×10^{-5}	0	0
KCl	$MgCl_2$	0.3931	-4.92×10^{-4}	0	0
KCl	UCl_3	-2.121	0.001491	1.569	-0.001689
KCl	UCl_4	-2.333	0.002062	0.5056	2.12×10^{-5}
KCl	KF	0.08214	-7.36×10^{-5}	0	0
KCl	ZrF_4	-1.906	6.93×10^{-4}	2.227	-0.001029
KF	LiF	-0.05708	2.90×10^{-5}	0	0
KF	ZrF_4	-1.774	5.79×10^{-4}	0.9944	-2.61×10^{-4}
LiCl	KCl	0.0768	-8.50×10^{-5}	0	0
LiCl	UCl_3	-1.525	0.001506	1.321	-0.001584
LiCl	UCl_4	-1.956	0.001796	1.404	-9.84×10^{-4}
LiF	BeF_2	-0.2616	7.53×10^{-5}	0	0
LiF	ThF_4	1.769	-0.001047	-1.798	8.73×10^{-4}
LiF	UF_4	2.219	-0.00177	-2.7853	0.002645
LiF	ZrF_4	-1.272	-4.87×10^{-4}	0.7348	2.31×10^{-4}
NaCl	$ThCl_4$	-0.2744	3.90×10^{-4}	0	0
NaCl	UCl_3	-0.1333	1.44×10^{-4}	0	0
NaCl	UCl_4	-2.8509	0.002824	3.025	-0.002985
NaCl	NaF	-0.117	1.77×10^{-5}	0	0
NaCl	ZrF_4	-1.0393	3.57×10^{-4}	-0.04282	1.84×10^{-4}
NaF	KF	-0.6499	2.97×10^{-4}	0	0
NaF	LiF	0.005952	-5.25×10^{-5}	0	0
NaF	ThF_4	0.4476	-7.62×10^{-4}	0	0
NaF	UF_4	-0.1274	-8.07×10^{-4}	0	0
NaF	ZrF_4	-1.2952	3.1×10^{-4}	-0.4568	6.65×10^{-4}
NaF	BeF_2	0.009154	-1.06×10^{-4}	0	0
UCl_3	UCl_4	0.1833	2.61×10^{-4}	0	0

Saline can read in the data from Tables 1 and 2, which are contained in .csv files in the GitLab project associated with MSTDB-TP. The MSTDB-TP developers plan to expand the number of pseudobinary systems evaluated for calculation of RK parameters. Moreover, the RK parameters will be continually updated as more duplicate pseudobinary datasets are evaluated, resulting in modifications in selected datasets incorporated into MSTDB-TP.

3. DATABASE TOOLS

Two tools have been developed to assist in the use of the database: an API called Saline and a GUI. Saline was developed to be a robust connection between MSTDB-TP to modeling and simulation codes, whereas

Table 2. Redlich–Kister parameters in MSTDB-TP v3.1 for viscosity estimation.

Salt 1	Salt 2	A_1^{12} (g/cm^3)	B_1^{12} (g/cm^3T)	C_1^{12} (g/cm^3T^2)	A_2^{12} (g/cm^3)	B_2^{12} (g/cm^3T)	C_2^{12} (g/cm^3T^2)
KCl	NaCl	1.931	-0.001878	0	-1.0121	-4.04×10^{-5}	0
KCl	$MgCl_2$	-4.258	0.005012	-1.66×10^{-6}	-6.125	0.009048	-3.00×10^{-6}
KCl	UCl_3	16.96	-0.0203	6.26×10^{-6}	-32.46	0.0400	-1.24×10^{-5}
KF	LiF	-0.6398	-2.80×10^{-4}	0	0	0	0
LiCl	KCl	-0.7936	6.61×10^{-4}	0	0	0	0
LiF	UF_4	-101	0.141	-4.71×10^{-5}	78.82	-0.1039	3.33×10^{-5}
NaF	KF	0.7318	-7.19×10^{-4}	0	-0.34734	5.99×10^{-4}	0
NaCl	$MgCl_2$	-0.1719	-7.55×10^{-4}	2.30×10^{-7}	-3.753	0.004986	-1.52×10^{-6}
NaCl	UCl_3	21.44	-0.02594	7.95×10^{-6}	-25.24	0.0301	-9.24×10^{-6}
LiCl	UCl_3	10.57	-0.01094	3.47×10^{-6}	-8.417	0.01062	-3.36×10^{-6}
NaCl	UCl_4	-4.008	0.005072	0	10.47	-0.008681	0
LiCl	UCl_4	-9.083	0.017	-5.65×10^{-6}	12.26	-0.01762	5.85×10^{-6}
KCl	UCl_4	-7.557	0.0132	-4.72×10^{-6}	20.08	-0.0267	9.52×10^{-6}
UCl_3	UCl_4	24.63	-0.02749	8.50×10^{-6}	17.13	-0.0208	6.42×10^{-6}
NaF	LiF	0.1938	-1.55×10^{-4}	0	0	0	0
NaF	UF_4	-130.6	0.1864	-6.44×10^{-5}	124.2	-0.169	5.72×10^{-5}
NaF	BeF_2	-97.66	0.1081	-3.29×10^{-5}	36.368	-0.0309	9.42×10^{-6}
LiF	BeF_2	-97.41	0.1043	-2.90×10^{-5}	104.354	-0.117	3.25×10^{-5}

the GUI was developed to make MSTDB-TP significantly more accessible to all types of users.

3.1 SALINE

Saline is the API providing programmatic access to the data provided by MSTDB-TP [17]. It is written in C++ and is provided as an open-source standalone library. Like many APIs, it is intended to insulate client software systems from knowing the details of the underlying data. Both Fortran and Python language bindings are provided to facilitate usage on machines from laptops to high-performance computing clusters.

Due to the tightly coupled development, updates during this FY primarily mirror those of MSTDB-TP. The most significant updates reflect the RK work of Section 2.3, overhauling the viscosity estimation implementation to utilize the newly developed parameters. Significant efforts have also been invested in the continuous integration and continuous delivery (CI/CD) process. The result of this effort is improved binary deployments, additional documentation, and new Python wheels for major operating systems. An example parity plot associated with this overhaul is shown in Fig. 5, which compares the RK estimated viscosity with measured values from specific compositions of NaCl-UCl_3 for which experimental data exist.

3.2 GRAPHICAL USER INTERFACE

The GUI was developed in Python to promote increased accessibility to MSTDB-TP data for all types of users. Currently, an executable file can be downloaded from the MSTDB-TP GitLab for Windows, but all operating systems will be supported in future iterations. The GUI allows the user to perform a wide variety of actions, including the following.

- Browse or search salts that are present in the database. Salts can be filtered by number of salt species (e.g., pure, binary, ternary) or by search term (e.g., "Cl," "F," "NaCl"). See the main window of the GUI in fig. 6.

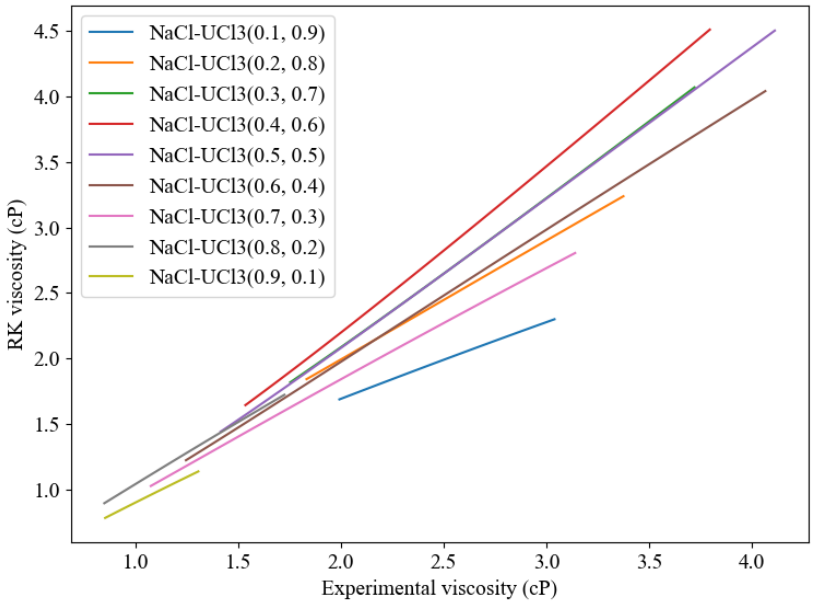


Figure 5. Example parity plot of RK-predicted viscosity versus the experimental measured viscosity for the NaCl-UCl_3 system, as calculated by Saline.

- Calculate TP properties (i.e., density, viscosity, thermal conductivity, and heat capacity) at a user-defined temperature for user-selected salt–composition combinations. Uncertainty, experimentally measured range, melting temperature, and boiling temperature are shown, along with the calculated properties.
- Plot TP properties for user-selected salts over either an experimentally measured range (automatic) or a user-defined temperature range (manual). See fig. 7 for examples.
- Use RK estimation models to calculate density for specific combinations of salts with the supported data. Binary and ternary plots can be produced. See figs. 8 and 9 for examples.

New additions from the past year include the estimation tool, which allows RK models to be used for the calculation of density. Endmembers from MSTDB-TP can be chosen, and binary–ternary combination density can be calculated and plotted. The salt selection window has also been updated with a "more info" button to show the original MSTDB-TP empirical parameters, fitting equation, and reference data.

3.3 MOLTEN SALT THERMAL PROPERTIES DATABASE WEBSITE

The MSTDB has a dedicated website where users can find information regarding both arms of MSTDB, access instructions, publications, contact information, and content from previous MSTDB workshops. The website can be accessed at mstdb.ornl.gov. A summary of the website's contents is given below.

- Links to both GitLab projects for each arm of the database for users who already have access.
- Specific instructions on how a potential user may acquire the appropriate qualifications for GitLab server access, as well as a link to a form that automatically generates a membership request.

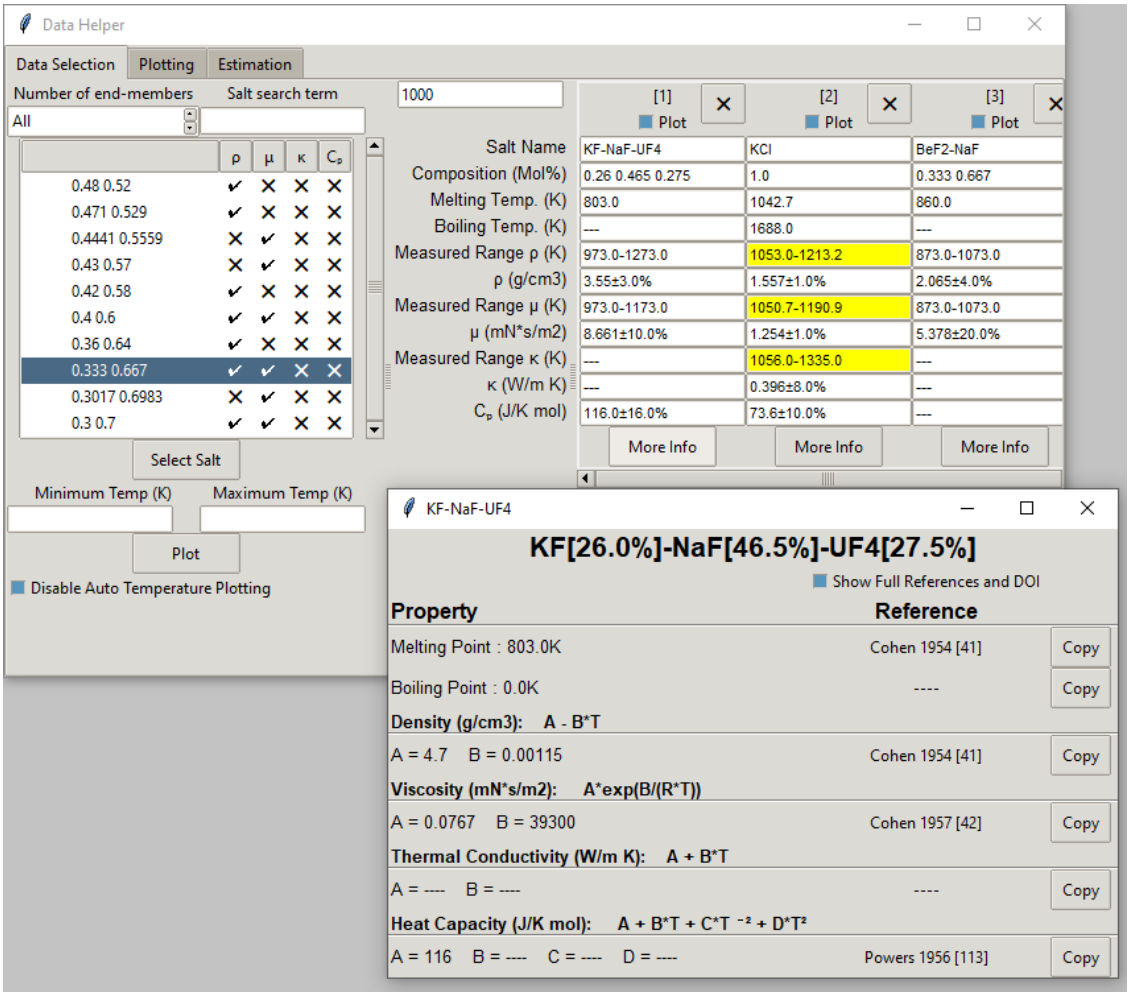


Figure 6. GUI main salt browse and selection screen

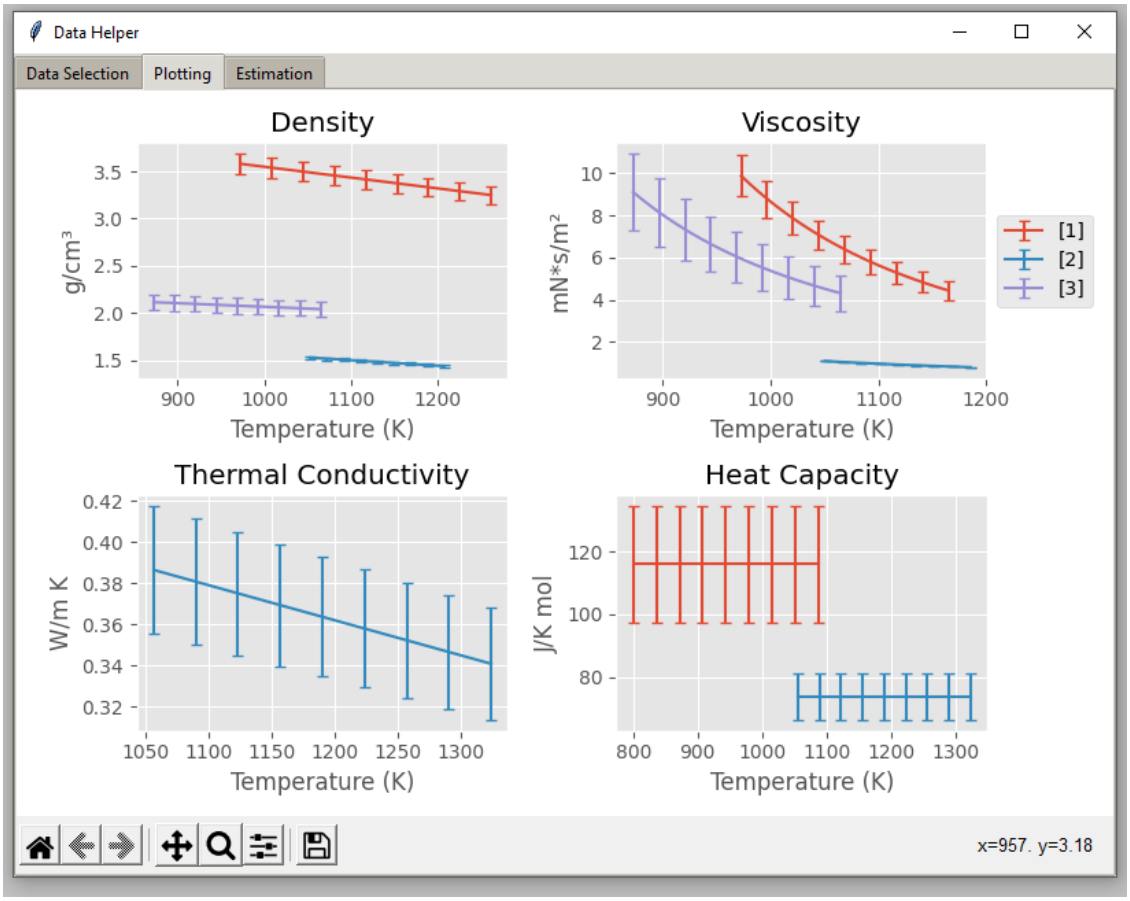


Figure 7. General plotting of MSTDB-TP experimental data.

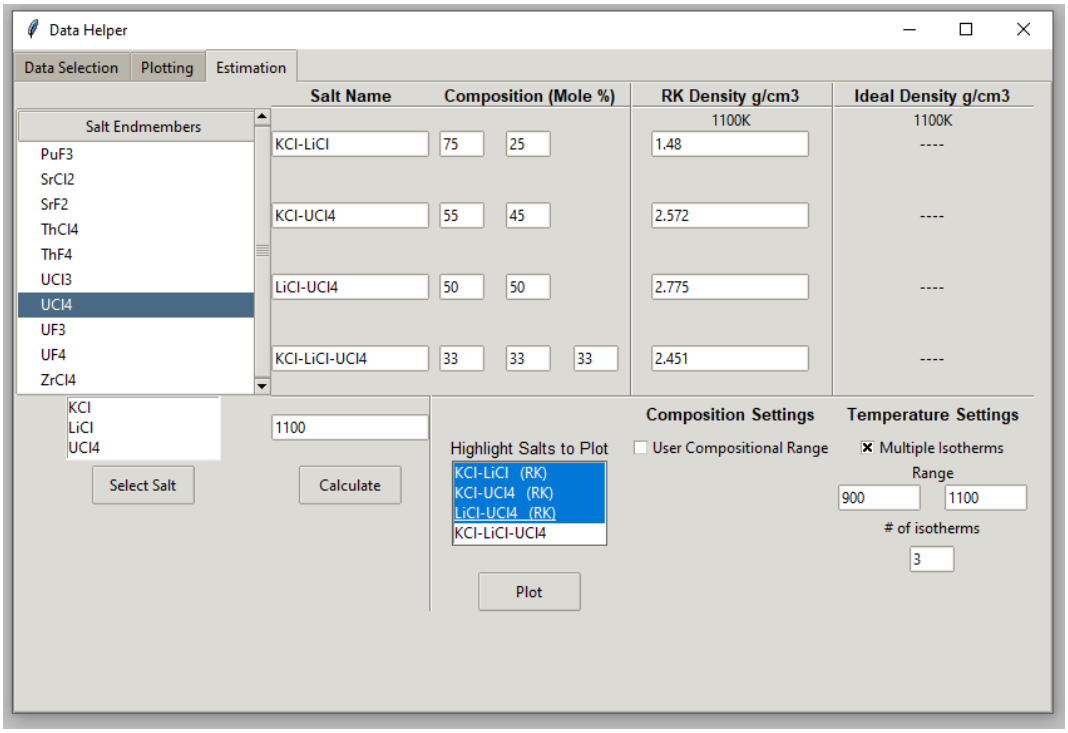


Figure 8. GUI's estimation tool main screen.

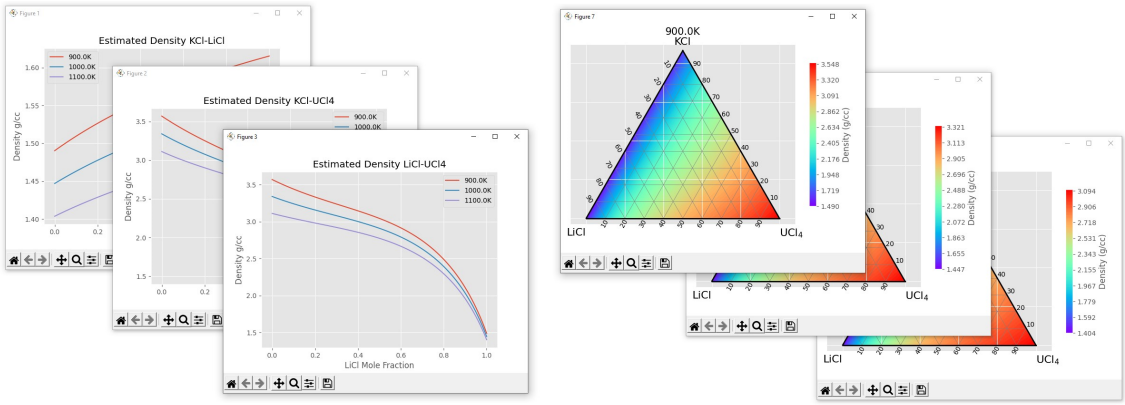


Figure 9. Binary and ternary plots of RK-estimated salts for multiple isotherms using the GUI's estimation tool.

- A description of the current state of MSTDB-TP, including information regarding the tools used to query the database.
- A description of the current state of MSTDB-TC, including compatibility notes regarding the usage of MSTDB-TC with state-of-the-art software.
- A complete list of publications related to both arms of the database, as well as links to all content for the 2020, 2021, 2023, and 2024 workshops.
- News articles related to key milestones associated with MSTDB.
- Contact information for all developers of MSTDB, both at ORNL and the University of South Carolina.

Additional information regarding MSTDB-TC can also be found on the website for the General Atomics Center for the Development of Transformational Nuclear Technologies: gacenterusc.org.

4. ONGOING AND FUTURE DEVELOPMENT OF MOLTEN SALT THERMAL PROPERTIES DATABASE–THERMOPHYSICAL

4.1 EXPANSION OF DATABASE TO INCLUDE SURFACE TENSION

Surface tension describes the cohesive forces between liquid molecules. Whereas molecules in the bulk interact equally with each other in all directions, surface molecules do not have the same neighbors on all sides. Therefore, a net inward force pulls the molecules toward the bulk, forming a "film" at the surface and restricting the ability of an object to pass through the interface compared to an object that is completely immersed. The same situation applies to the interface of immiscible liquids arising from differences in intermolecular forces at the contact surface. If the surface area of the liquid is increased, then work must be done for more molecules to be present at the surface, yielding an excess Gibbs energy relative to the interior of the liquid. Surface tension is the excess energy per unit area (force per unit length) with typical units of mN/m equivalent to dyn/cm. A linear relationship exists between surface tension and temperature, given by:

$$\gamma(T) = A - B * T(K) \tag{3}$$

When temperature increases, molecular thermal activity increases, which causes a decrease in the cohesive interaction and therefore surface tension.

Surface tension is another important thermophysical property to consider in the design and analysis of molten salt systems. It is especially important in determining the size, shape, and stability of bubbles and droplets. The breakup of falling streams into droplets is governed by Plateau–Rayleigh instability, which is a consequence of surface tension effects. It is also significant in the interface behavior of dissimilar liquids and emulsions. Surface tension may lead to the flotation of objects or particles more dense than the liquid. The curvature of a liquid's surface is determined by the surface tension and further impacts the contact angle with another surface, substantially affecting capillary action within tubes.

Several methods exist for measurement of surface tension, which can be grouped into force tensiometry and optical tensiometry [27]. Optical tensiometry is performed using a pendant drop shape analysis, where the shape of the drop is determined by a balance of forces, including the surface tension. This method allows for very small sample volumes (5–20 μL). Force tensiometry utilizes a probe connected to a very

sensitive balance, and the liquid interface is contacted with the probe. The size and shape of the probe are easily controlled and often made with platinum to ensure a zero contact angle between the probe and the liquid. Two probe configurations are commonly employed, the Wilhelmy plate and the du Noüy ring.

The du Noüy ring method utilizes a platinum ring as the probe. The liquid container is placed on a stage and positioned such that the ring is submerged below the interface. Then, the container is gradually lowered and the ring pulls through the interface, along with a meniscus of liquid. As the container is lowered further, the meniscus will separate from the ring. Prior to this event, the volume of the meniscus (and the force exerted) reaches a maximum value and begins to decrease before the separation occurs. The calculation of surface–interface tension depends on the maximum force measurement and does not consider the depth of the ring. However, small ring sizes can lead to a competing effect of capillary forces, which increases the measured surface tension. Correction factors may be utilized, which requires knowledge of fluid densities.

The Wilhelmy plate employs a rough platinum plate as the probe and considers the perimeter of the fully wetted plate contacting the liquid. The position of the plate relative to the liquid surface is critically important in this method. The instrument recognizes the exact moment of contact by a change in force on the probe, which is considered as zero immersion depth. The plate is immersed deeper, typically millimeters, and raised to the zero immersion depth, where force is again recorded.

These methods require a comparatively large amount of liquid (≥10 mL) to ensure complete wetting of the probe. Alternatively, a platinum rod can be employed in a cylindrical container utilizing the same methods and calculations as the Wilhelmy plate. Smaller vessels can be used, but care must be taken to ensure that vessel edges do not produce a meniscus within close proximity to the probe. The accuracy of the rod method depends on the certainty of the geometry and is typically less accurate than the plate method. Thus, this method is recommended only when sample volume is limited.

The most common method for surface tension observed in the literature of molten salts is the maximum bubble pressure method. This method involves submerging a capillary of known diameter into a molten salt and passing gas through to form bubbles (Figure 10). While attached to the capillary opening, the pressure inside the gas bubble increases. As the bubble size increases, the radius of curvature decreases (points A,B). Bubble pressure reaches a maximum value when the bubble forms a hemispherical shape with diameter equal to the capillary inner diameter (point C). The surface tension is determined through the reduced form of the Laplace equation, given by [1]

$$\gamma = \frac{\Delta P_{max} * R_{capillary}}{2}. \tag{4}$$

As the bubble grows beyond this point, pressure begins to decrease (point D). Finally, the bubble is detached from the capillary, and a new cycle begins (point E). This is a powerful method that does not require contact angle measurement—thus avoiding issues from surfactants or other impurities—has high accuracy and rapid performance time, and requires little liquid volume.

As demonstrated in Fig. 10, surface tension is an important factor in describing two-phase flow. Such flow regimes are highly influential in determining the thermal hydraulic behavior of fluid systems and may introduce dangerous situations such as impeded flow and local hotspots. These scenarios may occur as a result of normal operations such as entrainment of an inert cover gas or nuclear transmutation producing noble gases, or they could occur in an accident scenario such as a pipe break. Fluid interface behavior is also related to surface tension through various phenomena such as Rayleigh–Taylor instability. In the case

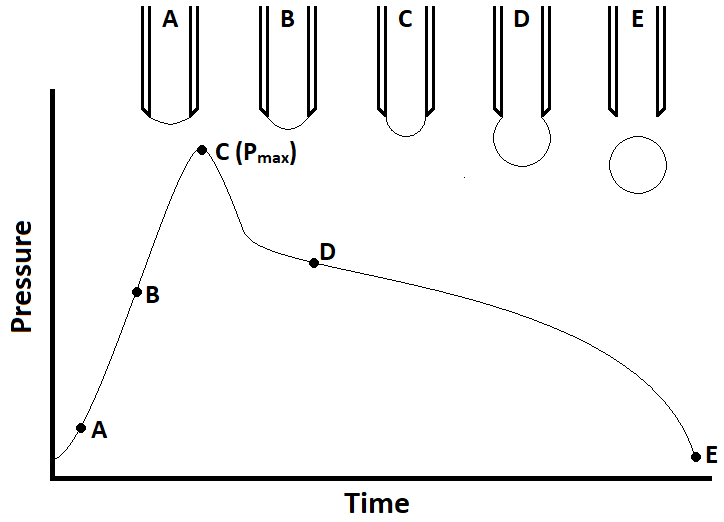


Figure 10. Pressure observed during bubble formation, growth, and detachment during surface tension measurement. Figure reproduced from Krüss Scientific [1].

of solid particles suspended in a fluid, surface tension is an important consideration in the balance of forces such as weight and buoyancy, added buoyancy from bubble attachment, and hydrodynamics [28]. Depending on which forces dominate this balance, different transport regimes may be observed.

Surface tension also indirectly affects the evaporation of molten salt and, therefore, equilibrium vapor pressure. Previous work has shown that cesium in a reactor coolant salt reduces the surface tension, causing an increase in the evaporation rate and forming a salt mist [29]. This phenomenon was observed in the Molten Salt Reactor Experiment. Salt mist formation is one mechanism by which radioactive contamination may be released to the environment in an accident scenario.

References for surface tension are currently being collected from published scientific literature. Many of the authors currently listed in MSDTB-TP have also published reports on molten salt surface tension measurements. These include Hara (1989) [30] , Katyshev (1980s – 2000s) [31] [32] [33], and Smirnov (1982) [34], as well as the molten salt property data compilations led by Janz (1960s–1980s) [35] [36] [37]. A significant amount of Russian literature was published in the 1940s–1960s. Some of these data are available in the context of refining metal slags. Much of the existing literature focuses on alkali and alkaline earth salts, whereas some later studies looked at actinide salts such as uranium and thorium [38].

The available data are then analyzed for reliability using a quality ranking system developed by Argonne that considers six factors [39]. These factors include method, calibrations, salt composition analysis, environmental controls, measurement precision, and verifiable property value. Each data resource is assigned a ranking of low, medium, or high quality across each of these six factors. These ranking are used to compare available data sets and select the most reliable correlation for inclusion in the MSTDB.

4.1.1 Future Plans for the GUI and Saline

The GUI is planned to be updated Current features under development include the following:

- Export tool: A tool to choose any combination of salt data within the database and compile it in

whatever format is useful to the user.

- Improvement to estimation tool: RK estimation is planned to be expanded to viscosity calculations. Thermal conductivity models are also planned for addition to the GUI as well (kinetic theory, etc.).
- Quality of life improvements such as advanced filters.

Saline development activities will continue to mirror MSTDB-TP activities, including the addition of interfaces and data structures to support surface tension data. There are also plans to support additional data formats and potentially additional estimation techniques. Further CI/CD work is also expected to simplify deployment to a variety of workflows, including those for researchers seeking to leverage AI technologies.

4.1.2 Investigation of Predictive Models for Thermal Conductivity

Thermal conductivity is a target property to be modeled predictively in the following fiscal year. However, it is a challenging property to model because of the severe lack of pseudobinary data available to formulate a RK-based approach. It is therefore necessary to use a more fundamental model that does not rely on mixture data to inform the non-idealities.

Some models have been developed and used with varying levels of success when applied to molten salts. Two models that treat the salt as a dilute gas are the Bridgman-type model [40], which considers dilute gas interactions in a cubic lattice and relates thermal conductivity to variations in free volumes/angles; and the Chapman–Enskog model [41], which models the energy transfer that occurs via collisions, modified with density and viscosity. Conversely, a phonon gas model developed by Zhao [42] describes thermal conductivity by phonon modes, approximated by macro-properties. Finally, Gheribi et al. have prescribed multiple iterations of a kinetic theory model [43, 44, 45, 46], accounting for complexation in later iterations.

One of the challenges with all of these models is that, in initial investigations, no model is generalizable to all possible salt mixtures, which exhibit varying degrees of complexation and ionic mass disparities. For example, actinide-bearing melts tend to have unrealistic kinetic theory estimations because the impact of the molar mass disparity has an over-damping effect on the thermal conductivity [47]. An example of this effect is shown for LiF-BeF_2-UF_4 in Fig. 11, where the models tend to under-approximate the thermal conductivity relative to experimental data [48].

Going forward, the MSTDB-TP developers intend to take inspiration from the aforementioned models that have been assessed for molten salt thermal conductivity and modify the approach such that the model can be generalizable for any salt that may exhibit full dissociation, complexation, polymerization, etc. This way, the model could be used for predictive capabilities in a manner similar to that of the RK methodology—but without relying on the pseudobinary mixture data to be fully fleshed out, since this is unlikely to happen experimentally within a reasonable timeframe for MSTDB-TP development considerations.

4.2 REQUEST MOLTEN SALT THERMAL PROPERTIES DATABASE MEMBERSHIP

The databases and associated documents are hosted on a publicly accessible, permission-protected server at ORNL: https://code.ornl.gov/neams/mstdb/. Access requires an account on the ORNL/ITSD GitLab server and an MSTDB membership, which, once granted, allows users to download all files.

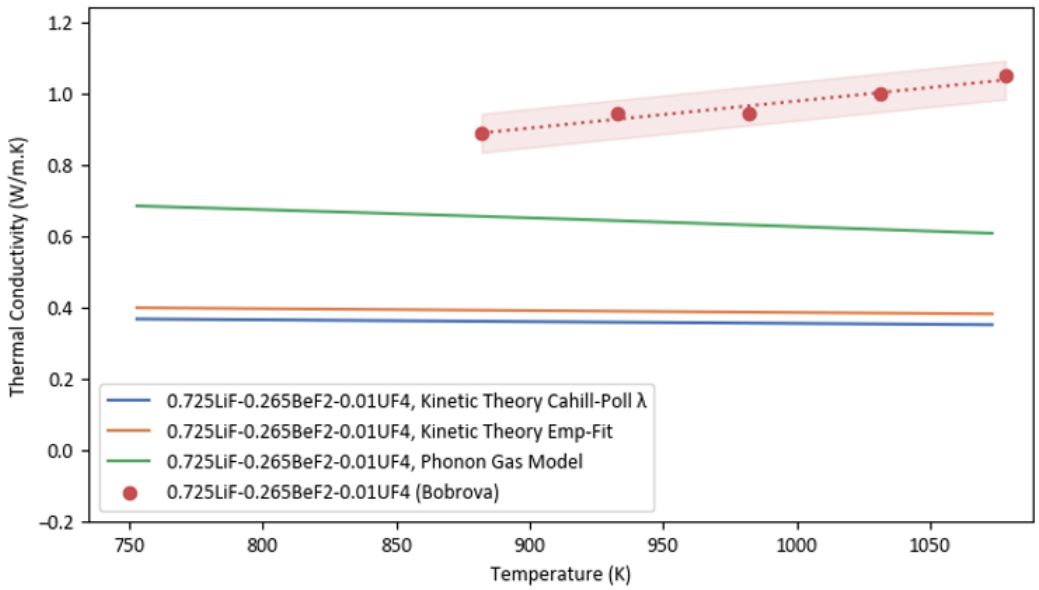


Figure 11. Predicted and measured thermal conductivity of LiF-BeF_2-UF_4.

ORNL is participating in OneID, an identity federation managed by DOE. ORNL employees can use the ORNL AzureAD login button for single sign-on, or the ORNL Yubikey login button to sign in with a certificate.

External collaborators can use the OneID login button to log in using an HSPD-12 PIV badge, a common access card (CAC), or credentials for one of the participating labs shown on the OneID screen. If you do not have a qualified badge or do not see your organization among the OneID choices, click the icon for Login.Gov and create an account. If you use the same email address for login.gov that you have registered in the past with XCAMS, your account will automatically be linked.

If you are logging into the GitLab server for the first time, be sure to take note of your username (e.g., @JohnDoe).

To Request MSTDB membership, please fill out the form at https://mstdb.ornl.gov/mstdb-signup/ with all necessary information. Doing so will notify the MSTDB team, and you will be added to the database on the closest Tuesday or Thursday relative to submission of the form.

If you are not automatically added to the GitLab project for MSTDB by the end of the closest Tuesday or Thursday relative to submission of the form, email mstdb@ornl.gov to inform that you have submitted the MSTDB sign-up form and you are awaiting access to the project.

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