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Quality Ranking of Unary Fluoride Salt Property Data in MSTDB-TP

Chemical and Fuel Cycle Technologies Division

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1. INTRODUCTION

Molten salt reactor developers rely on thermal property data to design, license and operate the reactors they are developing. The Molten Salt Thermal Database-Thermophysical Properties (MSTDB-TP) is being developed under the DOE Nuclear Energy Advanced Modeling and Simulation (NEAMS) program and managed by Oak Ridge National Laboratory. The MSTDB-TP is intended to serve as a single source of measured thermophysical property values for a wide variety of molten salt systems available to researchers, molten salt reactor developers, and regulators. These properties include melting and boiling points, heat capacity, density, viscosity and thermal diffusivity and conductivity.

Published measurements of molten salt properties are lacking for many salts and the data that are available are often inconsistent. This creates a challenge for MSR developers in determining which property values to select when designing their reactors. The MSDTDB-TP collects all available property data and down-selects to preferred data sets or correlations. It is the purpose of this work to apply a recently developed ranking system that indicates the quality of property values listed in the database to inform decisions about how to use the available data.

Quality assessments and rankings are being applied to data in MSTDB-TP to provide an indication of the quality of the data available. A previous report detailed the ranking system that was followed [1].

2. Quality Assessments

Each data set was evaluated by reviewing the source publication and assessing six aspects affecting data quality. The criteria in Table 1 were used to assess each aspect and a ranking was assigned to each criterion from the perspective of using the data for system design and licensing of an MSR. Each aspect was ranked as either high quality (H), moderate quality (M), or insufficient quality for quantitative use (I). An overall ranking was assigned to each data set based on the results of individual aspect rankings as below:

Rankings:

A Data ranked H or M for all quality criteria and verifiability ranked H

B Data ranked H or M for two or more quality criteria and verifiability ranked H or M.

C Property values calculated from models in the absence of measured values.

U* Data uncertainties do not warrant quantitative use of reported property value. However, all but the verifiability aspect are H or M.

U Data uncertainties do not warrant quantitative use of reported property value.

As an initial effort to document the quality of data in MSTDB-TP V2.1.0, all available sources of density, viscosity and thermal diffusivity or conductivity data for unary fluoride salts were reviewed and assessed.

Table 1: Quality Ranking Criteria for the Six Measurement Aspects [1]

Aspect	High Quality	Moderate Quality	Insufficient for Quantitative Use
Method	Standardized method for application to molten salts with international consensus	Well-established method being used at several laboratories	Documented procedure unique to small number of laboratories
Calibrations	Verification of proper instrument performance based on response of reference material *and* calibration of all devices and instruments used to determine property value with certified pure standards	Verification of proper instrument performance based on response of reference material *or* calibration of all devices and instruments used to determine property value with certified standards	Sufficient calibration results not provided
Composition	Replicate analyses of complete salt composition including cations, anions, and impurities, or controlled batching of known mixture under a controlled atmosphere	Replicate analysis for major cation salt constituents (typically > 3 mol %) and impurities prior to measurement	No analyses or only analysis for major cation salt constituents (typically >3 mol %) prior to measurement
Environmental Control	Confirmed control and stability of temperature and atmosphere during measurement	Measured salt or furnace temperature prior to measurement and limited control of atmosphere	Environmental controls not reported
Measurement Precision	Quantified uncertainty based on at least three replicate measurements	Propagated uncertainty or uncertainty budget based on individual measurements	No measured or estimated uncertainty are reported
Verifiability	Measured data and determined property value provided and verifiable	Both measured data and determined property value provided	Insufficient information available to verify reported value

3. Density

Available sources of measured density data for unary fluoride salts entered in the MSTDB-TP V2.1.0 were reviewed and assessed. Twenty-four individual sources of density data for unary fluoride salts were reviewed and assessed. Results of the assessments are compiled in Table 2, with short explanations for each aspect ranking. Eighteen of the sources used the hydrostatic method of measuring density, wherein a bob is suspended by a wire from a mass measuring device and the difference in mass when immersed is measured and used to calculate the density of the fluid. Six of the sources used a method of maximum bubble pressure, wherein the maximum pressure that can be sustained in a bubble of gas immersed in the fluid is measured and used to calculate density. Both of these methods are considered well-established due to frequent use, but neither has been standardized for use in molten salts. Many variations in the application of these methods to salts were found in the assessed literature. For example, the effect of the surface tension of the fluid interacting with the suspension wire was not always considered when determining the density using the hydrostatic method. Several authors noted effects on the measurement from persistent bubbles adhering to the bob and salt condensation on the support wire. It has not been standard practice to report the measured values from which density is calculated. In fact, only one source reported the measured differences in mass from which they calculated the density [13]. Therefore, most of the density values are ranked U or U* due to the verifiability category being ranked insufficient for quantitative use. This will alert users of the database that the density values cannot be verified using source data and should be used with caution.

Table 2. Quality Ranking of the Sources of Unary Fluoride Salt Density Data Compiled in MSTDB-TP V 2.1.0.

Author, Year [citation]	Salt Systems Studied	Overall Rank	Method	Calibrations	Composition Analysis	Environmental Controls	Measurement Precision	Verifiability
Jaegar, 1917 [2]	LiF, NaF, KF, RbF, CsF	**U**	**M** - Hydrostatic method	**M** - Measured a variety of organic liquids at RT, surface tension effect quantified ~0.0001 g/erg	**I** - No discussion of salt purity, source, or measurements of composition	**I** - No information provided on control of temperature or atmosphere	**M**- Reported accuracy to two decimal places in erg	**I** - No raw data provided, reports densities and a correlation
Edwards, 1953 [3]	NaF	**U**	**I** - Hydrostatic method, not enough detail to determine if method is correctly applied	**I** - No information provided on calibrations.	**I** - Salts were dried appropriately, No composition analysis	**I** - No information provided on control of temperature or atmosphere	**I** - No information on uncertainty or precision provided.	**I** - No raw data provided. Reports a correlation only
Yaffe, 1956 [4]	LiF, KF, CsF	**U**	**I** - Hydrostatic method, not enough detail to determine if method is correctly applied	**I** - No information provided on calibrations.	**I** - No information on source materials or analyses of salts.	**I**- No information provided on control of temperature or atmosphere	**I**- No information on uncertainty or precision provided.	**I** - No raw data provided. Reports a correlation and a standard deviation for the correlation.
Kirshenbaum, 1960 [5]	CaF_2, BaF_2, SrF_2, MgF_2, LaF_3, CeF_3	**U**	**M** - Hydrostatic method	**I** - No information provided on calibrations.	**M** - Salts dried appropriately, measured carbon, oxide and carbide post-test	**H** - Argon atmosphere, Temp controlled to ±15 K	**I** - Did not report measurement uncertainty, temperature uncertainty of 2 K.	**I** - No raw data provided. Reports measured density and a correlation.
Mackenzie, 1960 [6]	BeF_2	**U**	**M** - Hydrostatic method	**I** - Thermocouple calibrated to ±1 °C, no information on balance calibration	**M** - Salt impurities measured pre-test, appropriately dried, samples measured post test	**H** - Flowing inert atmosphere and temperature control of <2 °C	**M** - Report an uncertainty of single value at 800 °C,	**I** - Author notes results are approximate. Reports one measured value.
Kirshenbaum, 1961 [7]	ThF_4, UF_4	**U**	**M** - Hydrostatic method	**I** - Temperature was calibrated to 5 K, no information on balance calibration	**M** - Salts were appropriately dried and measured for impurities.	**H** - Temperature controlled to ±10 K, dry flowing argon atmosphere	**I** - Discussed sources of uncertainty and applied corrections, no uncertainty listed	**I** - No raw data provided. Reported measured density and a correlation.
Brown, 1964 [8]	LiF, NaF	**U***	**M** - Hydrostatic method, mass change measured by spring elongation	**H** - calibrated with KCl within an average deviation of ±0.4%	**M** - trace metal and oxygen content were reported pre-test, salts were vacuum dried	**H** - Conducted under helium purge, Temperature to ±1 °C	**H** - replicate measurements in both ascending and descending order, average deviation of ±0.4%	**I** - no raw data provided, reported correlation and method of least squares for fitting
Mellors, 1964 [9]	LiF, KF	**U**	**M** - Hydrostatic method, assumed effect of surface tension is negligible	**I** - No calibrations or uncertainty information reported	**I** - No composition analyses reported, no purification of salts reported	**H** - Conducted under a purified argon purge, Temperature to ±2 °C	**I** - No precision of measurements reported	**I** - No raw data provided; plots of measured values provided.

Table 2. Continued.

Author, Year	Salt Systems Studied	Overall Rank	Method	Calibrations	Composition Analysis	Environmental Controls	Measurement Precision	Verifiability
Porter, 1966 [10]	LiF, KF	**U**	**M** - Hydrostatic method, mass change measured by spring elongation	**M** - spring elongation constant uncertainty of ±0.1%. Density of bob measured to ±0.05%	**H** – Post-test analysis for oxygen and trace metals, Reagents vacuum dried	**I** - Helium purge**,** No reported uncertainty in temperature	**M** - ±0.1 %, measurements made at ascending and descending temperatures	**I** - No raw data provided, reported correlation and method of least squares for fitting
Hill, 1967 [11]	LiF, ThF_4	**U**	**M** - Hydrostatic method, not corrected for surface tension effect	**I** - No calibrations or uncertainty information reported	**M** - Appropriately dried salts, measured impurities pre-test. Analyzed for ThO_2 post-test	**H** - Temperature stabilized to ±0.2 °C, dry argon atmosphere	**I** – No uncertainty in measured density reported. Reported a standard deviation for the correlation	**I** - No raw data or measured densities provided. Report correlation by least squares.
Cantor, 1969 [12]	BeF_2	**U**	**I** - Hydrostatic method, persistent bubbles skewed results high	**I** - No calibration details for balances or with standard materials were reported	**M** – Pre-test trace metal and oxygen content reported, mixed salts were appropriately dried	**H** - Conducted under Ar purge (<5ppm H_2O), Temperature controlled to 0.2 °C	**M** - 0.4% reported uncertainty and a brief discussion of sources	**I** - No raw data or provided. Only reported correlation. Cautioned against quantitative use.
Fontana, 1970 [13]	NaF	**B**	**M** - Hydrostatic method, used post-test weight of bob to account for condensation	**I** -Temperature measured pre-test. No calibration of balance or measurement of standard fluids was reported.	**I** - No information on source materials or analyses of salts.	**I** - Purified Ar, no information on temperature control.	**M** - Report overall error < 0.2%, considered error in weighing, in initial mass, and surface tension effect	**H** – Reported raw data and calculated density as well as plots of measured density with correlations
Paucirova, 1970 [14]	LiF, NaF	**U**	**M** - Hydrostatic method, corrosion of the Pt wire in the gas phase was noted.	**I** - No information reported on calibrations	**I** - No information on source materials or analyses of salts.	**I** - No information reported.	**M** - Lists an accuracy of ±0.2%	**I** - No raw data provided. Report correlation constants only.
Mitchell, 1972 [15]	CaF_2	**U**	**M** - Hydrostatic method, used a weight transducer to measure change in mass as a force	**H** - Force measurement accuracy determined by deadweight loading to be 0.1% error. T control to ±10 °C (0.2% error)	**I** - No information on source materials or analyses of salts.	**I** - No information reported.	**I** - No precision of measurements reported	**I** - No raw data provided. Reported measured densities and correlations in a plot.
Smirnov, 1974 [16]	LiF, NaF, KF, RbF, CsF	**U**	**I** - No information provided.	**I** - No information provided	**I** - No information on source materials or analyses of salts.	**I** - Purified Ar, no information on temperature control.	**M** - Reported uncertainty < 0.003 g/cm^3	**I** - No raw data provided. Report correlation constants only.
Taniuchi, 1977 [17]	LiF, NaF, KF, BaF_2	**U**	**M** - Hydrostatic method with 2 bobs	**M** - Calibrated with distilled water and KNO_3.	**I** - Reagents dried appropriately- no measurement of impuritie reported.	**I** - Under flowing Ar, no information on temperature control.	**I** - Listed uncertainty for correlation constants, but not measured values.	**I** - No raw data provided. Reported measured density and correlation only.

Table 2. Continued.

Author, Year	Salt Systems Studied	Overall Rank	Method	Calibrations	Composition Analysis	Environmental Controls	Measurement Precision	Verifiability
Desyatnik, 1979 [18]	KF, UF_4	**U**	**M** - Maximum bubble pressure	**I** - No information on calibrations	**I**- No information on source materials or analyses of salts.	**I** - No information reported.	**I** - Reports a root mean square variance for the correlation	**I** - No raw data provided. Reports single density measurement and a correlation.
Desyatnik, 1981 [19]	NaF, KF, ThF_4	**U**	**M** - Maximum bubble pressure	**I** - No information reported on calibrations	**I** - Salts were dried appropriately, No composition analysis	**I** - No information reported.	**M**- Reported error <1%	**I** - No raw data provided. Reports correlations by least squares.
Smirnov, 1982 [20]	NaF, KF, RbF,	**U**	**M** - Capillary and Hydrostatic Methods	**M** - calibrated with KNO_3 and KCl	**I** - No composition measurement. Salts appropriately dried	**M** - Inert atmosphere, Temperature to 1 °C	**M** - 0.05% capillary, 0.04% Archimedes	**I** - No raw data provided. Reported correlation only.
Darienko, 1987 [21]	KF, HfF_4	**U**	**M**- Maximum bubble pressure	**I**- No information on calibrations.	**I** - Some salts were dried. No composition measurements.	**I** - Argon gas bubble, no information on temperature control.	**M** - Reported precision of <1%. Reported a standard deviation for the correlation.	**I** - No raw data provided. Reports correlations by least squares.
Katyshev, 1987 [22]	ZrF_4	**U***	**M** - Maximum bubble pressure	**M** - Manometer calibrated to ±0.015mm, micrometer to 0.01mm, no calibration of temperature or with standard fluids	**M** - Composition confirmed by chemical analysis post-test, Reagents appropriately dried	**H** - Details of Argon gas purification included, Temperature controlled to 2 °C	**M** - 1%	**I** - no raw data provided, Reports correlations by least squares.
Darienko, 1988 [23]	KF, ZrF_4	**U**	**M** - Maximum bubble pressure	**I** - No discussion of calibrations	**I** - Salts were dried and purified appropriately. No reported composition measurements	**I** - No information on control of atmosphere or temperature	**M** - Report a maximum relative error of 1–1.5%	**I** - No raw data provided. Reports correlations by least squares and a standard deviation.
Hara, 1989 [24]	LiF, NaF, KF, MgF_2, CaF_2, SrF_2, BaF_2	**U***	**M** - Hydrostatic method- with two bobs and Maximum bubble pressure method	**H** - Measured two samples of each salt, uncertainty in temperature as ±2 °C, measured mass as ± 1mg, and volume as ±0.0004 mL.	**H** - Salts were appropriately dried. Two samples of each salt were measured for impurities.	**H** - Temperature measured in-situ and controlled to ± 2 °C, under purified argon gas	**H** - A complete discussion of sources of error, reported total error ±0.22%, scatter in measured values is < 3.6%	**I** - No raw data provided. Tabulates correlation constants, shows measured density as points in plot.
Chen, 2002 [25]	CaF_2	**U**	**M**- Hydrostatic method	**I**- No information on calibration of temperature. Balance accuracy of 0.1 mg	**I** - Salts dried appropriately. No direct measurements of composition	**H** - Dry flowing argon. Temperature was controlled to ±5 K	**H** - Balance accuracy of 0.1 mg, reported relative error of ±0.2%, total uncertainty reported at <1%, performed two sets of measurements.	**I** - No raw data provided. Measured densities plotted. Reported a correlation.

4. Viscosity

Available sources of measured viscosity values for unary fluoride salts entered in the MSTDB-TP V2.1.0 were reviewed and assessed. Eight individual sources of viscosity data for unary fluoride salts were reviewed and assessed. The results of these assessments are compiled in Table 3, with short explanations for each aspect ranking. Five of the sources used the oscillating crucible method of measuring viscosity, wherein a crucible of salt is suspended by a wire and oscillated and the measured damping due to the molten salt in the crucible is used to calculate the viscosity of the fluid. One of the sources used a rotational method, in which a cylindrical spindle is immersed in molten salt and the torque required to rotate it at a particular speed is measured and used to calculate the viscosity. Two sources did not provide any information on the method used or cited sources that were inaccessible. It has not been standard practice to report the measured data from which viscosity is calculated. Therefore, all the sources are ranked U or U* due to the verifiability category being ranked insufficient for quantitative use. This will alert users of the database that the viscosity values have not been verified and should be used with caution.

Table 3: Quality Ranking of the Sources of Unary Fluoride Salt Viscosity Data Compiled in MSTDB-TP V 2.1.0.

Author, Year	Salt Systems Studied	Overall Rank	Method	Calibrations	Composition Analysis	Environmental Controls	Measurement Precision	Verifiability
Moynihan, 1968 [26]	BeF_2	**U***	**M** - Rotational viscometer	**M** - calibrated with two NBS standard oils at room temperature	**M** - Salts dried appropriately. Reported trace metal and oxygen content pre-test.	**H** - Conducted under dry helium in a glovebox, Temperature controlled to 0.2 °C	**H** - ±3% uncertainty and reported quantified uncertainty from individual sources	**I** - No raw data provided.
Smirnov, 1974 [16]	LiF, KF, NaF, RbF, CsF	**U**	**I** - No information provided.	**I** - No information on calibrations provided	**I** - No information on source materials or analyses of salts.	**I** - Purified argon atmosphere. No information about temperature control.	**I** - Reported standard deviation of all measurements <0.015 cP	**I** - No raw data provided. Reported correlation only.
Desyatnik, 1978 [27]	LiF, KF, UF_4	**U**	**M** - Oscillating crucible method	**I** - No information on calibrations provided	**I** - Salts appropriately dried. No composition measurements.	**I** - Purified argon atmosphere. No information on temperature control.	**M** - Reported a coefficient of variation as 2.0%.	**I** - No raw data provided. Reports correlations with standard deviations.
Abe, 1981 [28]	LiF	**U**	**M** - Oscillating Crucible Method	**I** - No information on calibrations provided	**M** - Salts were dried and purified appropriately. No composition measurements reported.	**I** - Crucible is welded shut with salt inside under vacuum. No information on temperature control.	**H** - Uncertainty <±0.9%. Analyzed individual sources of uncertainty. Measurements at both ascending and descending temperatures	**I** - No raw data provided. Reports average viscosity at each temperature and a correlation.
Desyatnik, 1981 [19]	NaF, KF	**U**	**M** - Oscillating crucible method	**I** - No information on calibrations provided	**I** - Salts dried appropriately. No direct measurements of composition	**I** - Purified argon atmosphere. No information on temperature control.	**M** - Reported error of 2.0%	**I** - No raw data or measured viscosity reported. Report the coefficients of a correlation.
Nguyen, 2000 [29]	LiF, KF	**U**	**M** - Oscillating Crucible method (Torsion Pendulum)	**I** - No information on calibrations provided	**I** - Salts dried appropriately. No direct measurements of composition	**I** - Glovebox with dry inert atmosphere. No information on temperature control.	**M** - Report error as <2%	**I** - No raw data provided. Report viscosity and correlation.
Kubikova, 2008 [30]	NaF, KF	**U**	**I** - cites other work which is not available for the method	**I** - No information reported on calibrations	**I** - Salts dried appropriately. No composition measurements.	**I** - Glovebox with dry N2 atmosphere. No information on temperature control.	**M** - maximum uncertainty reported as ± 0.02 mPa s. Reports standard deviation for the correlation constants.	**I** - No raw data provided. Reports measured viscosities and correlation in a figure and table.
Takeda, 2015 [31]	MgF_2, CaF_2, SrF_2, BaF_2	**U**	**M** - Oscillating Crucible Method	**I** - No information on calibrations.	**M** - Salts were dried appropriately. Reported 99.9% purity.	**H** - Temperature controlled to 0.5 K, dry helium atmosphere with Zr sponge.	**M** - total error is 3%, quantified individual sources of error.	**I** - No raw data provided. Reported measured viscosities and a correlation fit using least squares.

5. Thermal Diffusivity and Conductivity

Available sources of measured thermal diffusivity and conductivity data for unary fluoride salts in the MSTDB-TP V2.1.0 were reviewed and assessed. Six individual sources of viscosity data for unary fluoride salts were reviewed and assessed. The results of these assessments are compiled in Table 4, with short explanations for each aspect ranking. Various methods were used to measure the property values. Some sources measured thermal diffusivity and calculated thermal conductivity while others measured thermal conductivity directly. Two sources did not report measured values, but provided modeled values based on measurements of other salts or first principles. These sources are marked with a rank of C to indicate computational results. This will alert users of the database that these values are not based on measurements. It has not been standard practice to report the data from which the thermal diffusivity or conductivity value is calculated. Therefore, many of the sources are ranked U due to the verifiability category being ranked insufficient for quantitative use. This will alert users of the database that the property values are not verified and should be used with caution.

Table 4: Quality Ranking of the Sources of Unary Fluoride Salt Thermal Diffusivity and Conductivity Data Compiled in MSTDB-TP V 2.1.0.

Author, Year	**Salt Systems Studied**	**Overall Rank**	**Method**	**Calibrations**	**Composition Analysis**	**Environmental Controls**	**Measurement Precision**	**Verifiability**
Sreenivasan, 1967 [32]	LiF	**B**	**M** - Transient Gap Analysis	**M** - Calibrated with sodium nitrate, microvolt amplifier ±0.4 µV and recorder ±0.5 µV	**I** - LiF purchased at 99.989% pure, no composition measurements	**M** - Under argon atmosphere, platinel thermocouples used but did not quantify stability	**H** - Replicate samples, quantified error for measurements of each sample. Uncertainty of the technique is estimated at 8.6%	**H** - Reports raw data and calculated values. Reports a correlation by least squares and its maximum deviation from measured values.
Powell, 1979 [33]	CaF_2	**U**	**M** - Hot Wire	**M** - calibrated with organic liquids at RT, current stabilized to 0.0001 amps	**I** - No information on source materials or analyses of salts.	**I** - No information reported.	**I** - Provided discussion of sources of error, 1024 data points are smoothed by averaging every 16 data points	**I** - No raw data provided. Reported two measured values in plot, and correlation generated by least squares.
Smirnov, 1987 [34]	LiF, NaF, KF, RbF, CsF	**U**	**M** - Coaxial cylinders	**M** - Maximum measurement error of 4%	**I** - Salts purified by zone melting - no composition analyses	**M** - Temperature controlled to 0.01 K, sealed in an air tight container- did not reported cover gas	**I** - no information reported	**I** - No raw data provided. Report measured conductivity and correlations which match the measured values within 5%.
Golyshev, 1992 [35]	LiF, MgF_2, BaF_2, CaF_2	**U**	**M** - Coaxial Cylinders	**I** - No information on calibrations.	**I** - No information on source materials or analyses of salts.	**I** - No information reported.	**M** - Measured 2–4 replicate cells. Error in averaging is estimated at 0.2%	**I** - No raw data provided. Reports measured diffusivity on a plot.
Nagaska, 1993 [36]	LiF, NaF, KF, RbF, CsF	**C**	**I** - Measured non-fluoride salts by Rayleigh scattering and predicted fluoride conductivity	**I** - n/a	**I** - n/a	**I** - n/a	**I** - n/a	**I** - Reported a correlation for fluorides based on measurements of non-fluoride salts
Gheribi, 2014 [37]	LiF, NaF, KF, RbF, CsF, MgF_2, CaF_2, BaF_2	**C**	**I** - Did not measure values- computational work only	**I** - n/a	**I** - n/a	**I** - n/a	**I** - n/a	**I** - generated correlations for fluorides based on modeling

6. Summary

Thirty-six available and accessible sources of property values for the density, viscosity and thermal diffusivity and conductivity of unary fluoride salts in MSTDB-TP V2.1.0 were reviewed and assessed for quality. Overall rankings were assigned to provide database users with an indication of the reliability of the property values for use in design and licensing. This assessment was limited to property values included in MSTDB-TP V2.1.0. Subsequent releases of the database with additional values will require review and assessment of those data sets. As standardized methods of measuring the properties of molten salts become available, existing data should be re-evaluated.

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