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Uncertainty in Molten Salt Properties

MSR Developer Conference 2022

Melissa A. Rose
Chemical and Fuel Cycle Technologies Division
Argonne National Laboratory

Molten Salt Reactor PROGRAM

Provide the data necessary to build a FOAK MSR by 2035

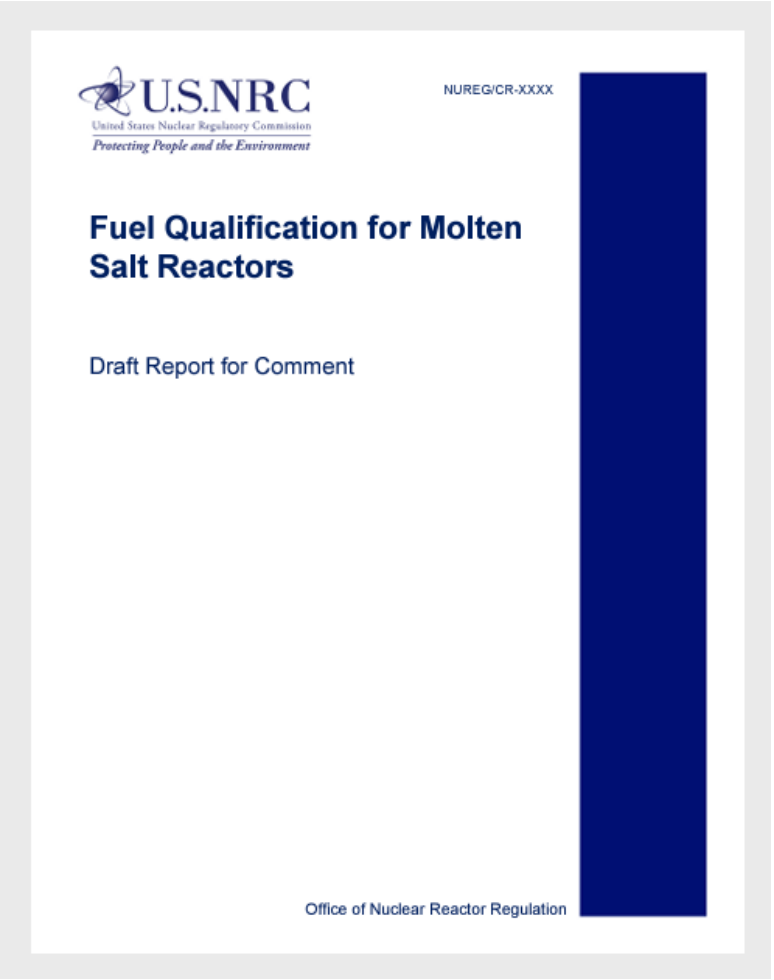
NQA-1 quality data will likely be necessary for licensing a reactor

- Use of standardized methods
- Precision and accuracy of analyses determined based on measurements with reference salts
- Measured under a quality assurance program

Property data used for licensing must have well defined levels of uncertainty

Sources of uncertainty in measurements can include:

- Instrumental limitations and calibration
- Use of an inappropriate measurement method
- Improper application of measurement method
- Inadequate control of environmental conditions
- Salt Composition, trace contamination



*Understanding the relationship between fuel salt composition and properties is key to fuel salt qualification.– **Draft Report on MSR Fuel Salt Qualification***

Impact of Uncertainty on Modeling

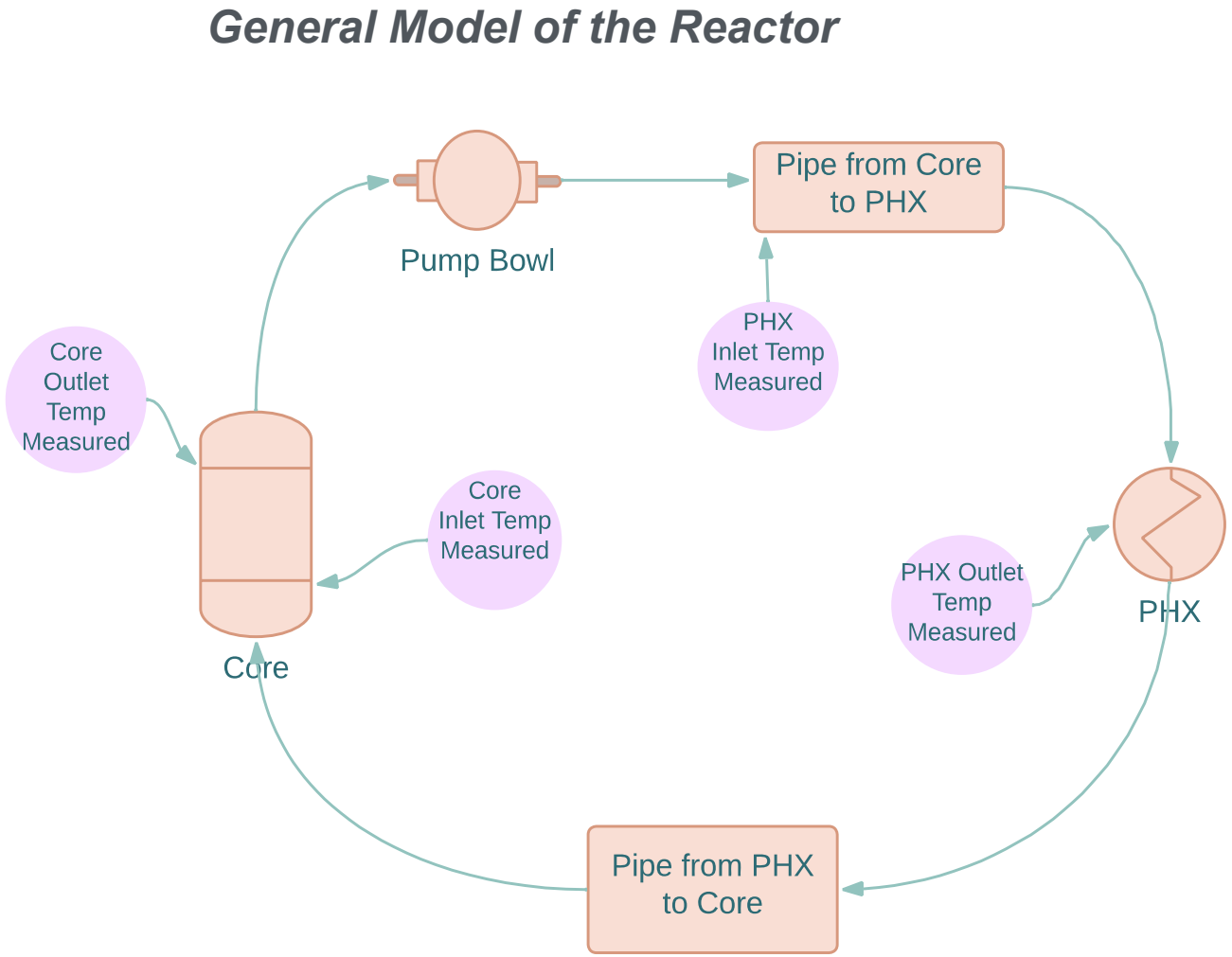
A Parametric Study

- Need to understand how uncertainty in molten salt property values will impact modeling predictions
  - Uncertainty in measured property values
  - Salts that are multicomponent near-eutectic mixtures
  - Fission product accumulation during operation that change salt compositions

- Conducted a parametric study using a combined uncertainty to represent the above factors and examine the effect on model results

Parametric Study

- A Molten Salt Demonstration Reactor (MSDR) model was used by applying TRANSFORM to a steady-state case
  - LiF-BeF_2-ThF_4-UF_4 (71.5-16.0-12.0-0.5 mole %) fuel salt was used in the model calculations
  - Credit: Sara Creasman of University of Tennessee Knoxville
  - Report ANL/CFCT-22/17 describing this study was released in August



Parametric Study

- Range of individual property values around mean used to examine the change in four output temperatures from the base case

Range of Property Values Used

Property	Low Uncertainty	Mid-Uncertainty	High Uncertainty
Density	± 5 %	± 10 %	± 20 %
Heat Capacity	± 5 %	± 10 %	± 20 %
Thermal Conductivity	± 5 %	± 10 %	± 20 %
Viscosity	± 5 %	± 10 %	± 20 %

Base Case Property Values for $LiF\text{-}BeF_2\text{-}ThF_4\text{-}UF_4$ (71.5-16.0-12.0-0.5 mole %) fuel Salt [1].

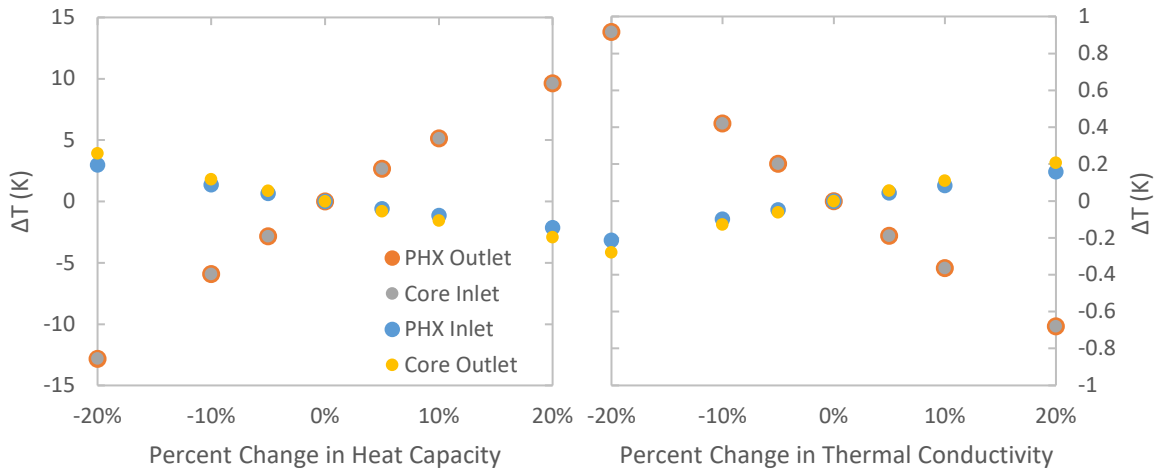
Property	Units	Baseline Value or Correlation
Melting Temp	K	773
Density	lb/ft^3	236.3 - 0.0233 T(°F)
Thermal Conductivity	Btu/hr-ft-(°F)	0.75
Specific Heat Capacity	Btu/lb-(°F)	0.32
Viscosity	lb/hr-ft	$0.2637\ e^{(7362\ /\ (459.7\ +\ T(°F)))}$

[1] Bettis, E. S., L. G. Alexander, and H. L. Watts. Design Studies of a Molten-Salt Reactor Demonstration Plant. No. ORNL-TM-3832. Oak Ridge National Lab., Tenn., 1972.

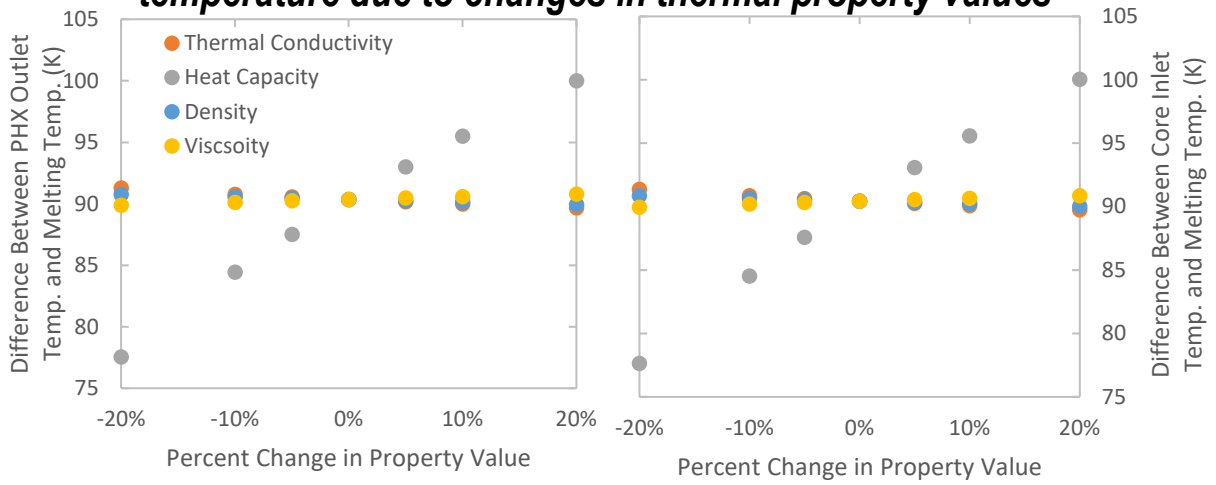
Response to Changes in Property Values

- Value of heat capacity has the largest effect, followed by thermal conductivity
- Thermal conductivity trends are the reverse of heat capacity
- Examined how close changes to property values brought the output temperatures to the melting temp (773 K)
  - The lowest heat capacity resulted in a calculated salt temperature only 77 K higher than the freezing temperature

Change in output temperatures due to changes in thermal property values



Difference between out temperatures and nominal melting temperature due to changes in thermal property values



Key Findings of the Parametric Study

Key findings:

- Model results are sensitive to property values
- Variance in heat capacity is the most impactful
- Sensitivity indicates required precision levels for property measurements, which prioritizes method development
- Accurate prediction of melting temperatures needed for reliable operation

Future studies should evaluate:

- Effect of uncertainties in the temperature dependence of property values on model predictions
- Combined effects of property values on model predictions
- Models of reactors for transient conditions

Incorporation of these additional factors will more accurately quantify the sensitivity of modeling predictions to uncertainty in molten salt property values

Quality Assessment and Ranking Approach for Databases

Goal: To provide developers with a complete and transparent assessment of the quality of molten salt property data in the MSTDB

Assessed applicability of quality assessment methods used for existing property databases

- International Center for Diffraction Data Powder Diffraction File for X-ray diffraction data
- International Union of Pure and Applied Chemistry - National Institute of Standards and Technology Solubility Data Series for solubility data
- Recent critical evaluations of property data for several molten salts available in the open literature [1]

Common features of existing databases include:

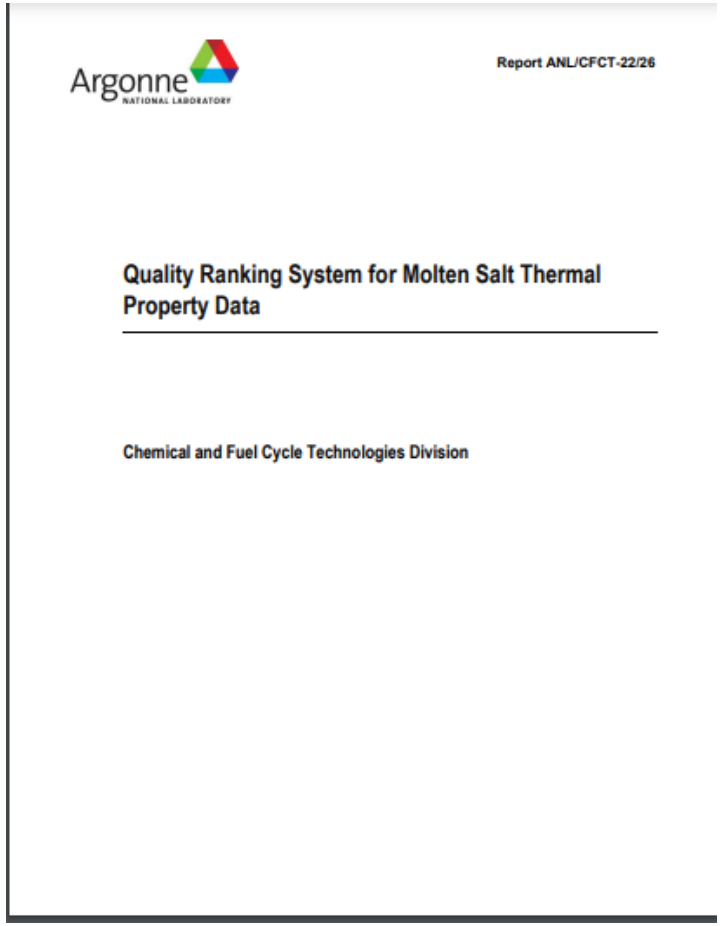
- Retention of all existing data sets, not only the single "best" data set
- Detailed bibliographic and experimental information
- Detailed history of assessments of each data set
- A ranking is applied to each data set based on the assessment

[1] K. Tasdou, J. Magnusson, T. Munro and M.J. Assael (2019). "Reference Correlations for the Viscosity of Molten LiF-NaF-KF, LiF-BeF2, and Li2CO3-Na2CO3-K2CO3." *J. Phys. Chem. Ref. Data. Vol 48.* 043102.

Property Data Assessment

Recommend an assessment across six aspects for existing and new data for the MSTDB-TP:

1. Method
   Appropriate and applied correctly, ideally a standardized method
2. Calibrations
   Verified instrument performance with certified standard materials
3. Salt Composition Analysis
   Replicate analyses including anion and impurity concentrations
4. Environmental Controls
   Control and stability of temperature and atmosphere
5. Measurement Precision
   Uncertainty quantified with at least three replicate measurements
6. Verifiability of Property Determination- capstone criterion
   Value can be independently verified from the reported data


Argonne NATIONAL LABORATORY

Report ANL/CFCT-22/26

Quality Ranking System for Molten Salt Thermal Property Data

Chemical and Fuel Cycle Technologies Division

Recently released report on data quality assessment and ranking approach: ANL/CFCT-22/26

Ranking Approach

Datasets are ranked as either high quality (H), moderate quality (M) or incomplete (I) with regard to each of the six aspects.

Overall Rankings for Data Entries then depend on these six aspect assessments:

A. Data is ranked H or M for all quality aspects and property verification ranked H
B. Data ranked H or M for two or more quality aspects and property verification ranked H or M.
U. Data uncertainties do not warrant quantitative use of reported property value.

Notes on application to MSTDB:

- Should be applied to both new and existing data sets
- Highest ranked data set can be identified in the database

Summary

NQA-1 quality level data with well-defined uncertainty will likely be required to license molten salt reactors

A parametric study assessing the sensitivity of modeling MSRs to key property values showed heat capacity value to be most impactful during steady-state operation

Recommended a quality assessment and ranking approach for publically available DOE-NE managed databases

Acknowledgements

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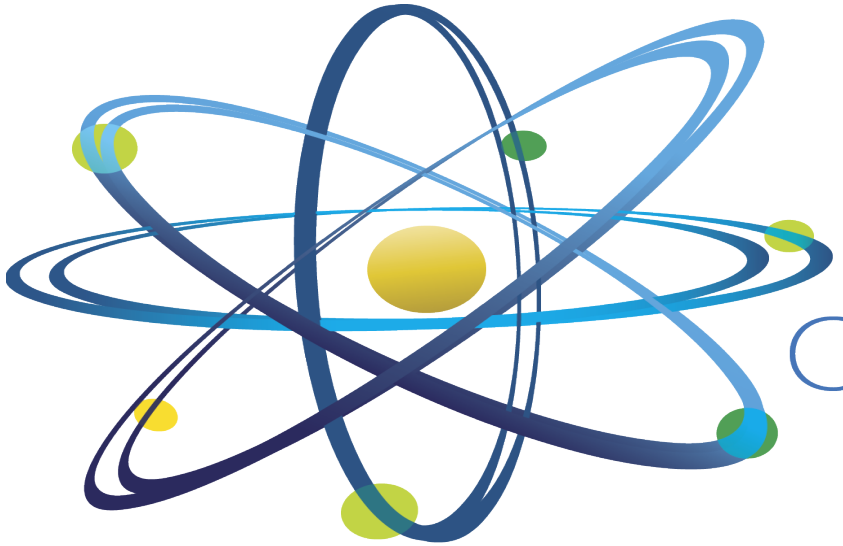
Questions



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marose@anl.gov

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