KNS Autumn Meeting · Gyeongju · October 29–30, 2026

Quality-Weighted Thermophysical Property Database and Uncertainty Quantification for Molten Salts

2026 Undergraduate Global research team (Hanuel Park, Dongwoo Lee, Woosung Joo, Chanyeong Choi, Yejun Han, Junsu Bang), RA Chaehyun Kim
Prof. Yong Hoon Jeong

Department of Nuclear and Quantum Engineering,
Korea Advanced Institute of Science and Technology

Contents

01 Background and motivation

02 Scope and flow

03 Database construction

04 Quality scoring framework

05 Two-stage prediction & uncertainty

06 Demonstration & leave one out check

07 Conclusions

08 Acknowledgements

Introduction

Property uncertainty in candidate molten salts is not a single number; correlations disagree across the literature, and the disagreement shifts peak temperatures, response times and return-to-steady margins in transient safety problems. The work treats this chain quantitatively across a database, a quality-weighted procedure and demonstrations.

THE CHAIN

Property → physics → margin

— correlation spread in the literature

— shifts peak T, response, return-to-steady

— quantified, not assumed away

THE PROGRAMME

Joint work, for advisory and industrial view

— DTU advisory · Saltfoss Energy industrial view

— KAIST lead execution

Research flow

WP 1

Property database v1.0

Curated thermophysical source database

— 32 source correlations

— 4 salts × 4 properties

— JSON, provenance, range, u

IN THIS PRESENTATION

WP 2

Surrogate & stability

Fits, composition, stability matrix

— temperature-dependent fits

— error propagation

— chemical-stability matrix

IN THIS PRESENTATION

WP 3

Reduced-order model

Compact neutronics + thermal-hydraulic

— six-group point kinetics

— 1D nodalization

— baseline validated

FOLLOW-ON

WP 4

Transient scenarios

Four representative transients

— load follow

— loss of flow

— reactivity insertion, inlet-T

FOLLOW-ON

WP 5

Envelope & release

Safety-envelope map, dissemination

— salt-by-salt map

— 2+ conference papers

— open release

FOLLOW-ON

Database construction

50+ literature sources reviewed; duplicates and correlations with excessive reported error removed during screening; 32 source correlations retained and stored as JSON records.

TABLE · CORRELATION COUNTS BY SALT AND PROPERTY

SALT SYSTEM	DENSITY	VISCOSITY	SPECIFIC HEAT	CONDUCTIVITY
FLiBe	4	7	3	1
FLiNaK	4	4	2	1
$NaF–KF–UF_4$	3	4	2	1
$MgCl_2–KCl–NaCl$	6	4	4	4

SCOPE

50+ → 32

sources reviewed, retained after duplicate filtering.

Scoring criteria – 3 categories, kept independent

Each source correlation is scored by three quantitative criteria. They are not collapsed into a single rating, and they are not assumed equally informative.

CRITERION 1

Reported error

Measurement uncertainty and fitting error of the source, on a common standard-uncertainty basis.

CRITERION 2

Supporting evidence

Number of experimental data points, log-compressed so a 10–100 gap counts more than 1000–1100.

CRITERION 3

Cross-study agreement

Mean pairwise deviation against overlapping correlations, pointwise.

Score definitions and agreement

Error-based sub score(for both exp/fit)

Within each salt–property group, smallest error maps to 1, largest to 0.

$$S_{E,i} = (E_{max} - E_i) / (E_{max} - E_{min}) \quad (1)$$

Combined error-based score

Adjustable α-split; default 1/2 when both quantities reported.

$$S_{err,i} = \alpha_{exp} S_{exp,i} + \alpha_{fit} S_{fit,i} \quad (2)$$

Data-point score

Logarithmic compression; missing counts reweighted through available criteria.

$$S_{N,i} = \ln(1 + N_i) / \ln(1 + N_{max}) \quad (3)$$

Consistency score

Pointwise, with mean magnitude in the denominator.

$$d_{ij,k} = |y_{i,k} - y_{j,k}| / ((|y_{i,k}| + |y_{j,k}|)/2) \quad (4)$$

$$D_i = (1/M_i) \sum_{j \neq i} (1/K_{ij}) \sum_k d_{ij,k}, \quad S_{cons,i} = (D_{max} - D_i) / (D_{max} - D_{min}) \quad (5)\text{–}(6)$$

Composite quality and relative weights

Three criterion scores combined into one composite, then normalized within each salt–property group to produce a weight that sums to one.

Composite quality score

Coefficients sum to one; default 1/3 each during demonstration.

$$Q_i = w_{err}\, S_{err,i} + w_N\, S_{N,i} + w_{cons}\, S_{cons,i} \tag{7}$$

Relative quality weight

Within-group normalization; $\Sigma W_i = 1$.

$$W_i = Q_i / \Sigma_j Q_j,\ \Sigma W_i = 1 \tag{8}$$

EXAMPLE · FLiBE DENSITY

Reported errors 0.8 / 1.5 / 2.5 / 4.0% → scores 1.000 / 0.781 / 0.469 / 0.000 under Eq. (1), then reweighted to a vector summing to one.

Predicting at an unmeasured composition

When no source has measured the composition of interest, we predict from representatives that were constructed at neighboring measured compositions. The interpolation coefficients depend only on the position of the target relative to the measured neighbors, and they sum to one.

COMBINED REPRESENTATIVE

Predicted value at composition x*

Eq. (11) · sum of weighted representatives around x*

$$\hat{y}(T, x^*) = \Sigma r\ \lambda r(x^*)\tilde{y}r(T)$$

Each $\tilde{y}_r(T)$ is the representative already constructed for measured composition r. Coefficients $\lambda_r(x^*)$ sum to one. Quality weights do not enter this step; the operation is purely geometric.

BINARY LINEAR FORM

$$\lambda 1 = (x2 - x^*) / (x2 - x1),\ \lambda 2 = (x^* - x1) / (x2 - x1)$$

Closed-form coefficients when two measured compositions bracket the target.

Uncertainty propagation

Reported uncertainty and fitting error converted to a common basis, propagated through weighting, the refit and composition interpolation.

Combined source uncertainty

Squared sum under independence; missing component dropped.

$$u_i^2 = u_{meas,i}^2 + u_{fit,i}^2 \tag{14}$$

Representative uncertainty

Renormalized weights squared; refit residual added separately.

$$u_r^2(T) = \sum_i \omega_{i,r}^2(T)\, u_i^2(T) + u_{repfit,r}^2(T) \tag{15}$$

Interpolation uncertainty

Composition interpolation propagates the same variances; in binary: convex sum.

$$u_{pred}^2(T, x*) = \sum_r \lambda_r^2(x*)\, u_r^2(T)$$
$$u_{pred}^2 = \lambda_1^2\, u_1^2 + \lambda_2^2\, u_2^2 \tag{16), (17}$$

Approximate uncertainty interval

The combined standard uncertainty u_{pred} is reported as an approximate two-sided interval around the predicted value, under a normal approximation.

GENERAL FORM

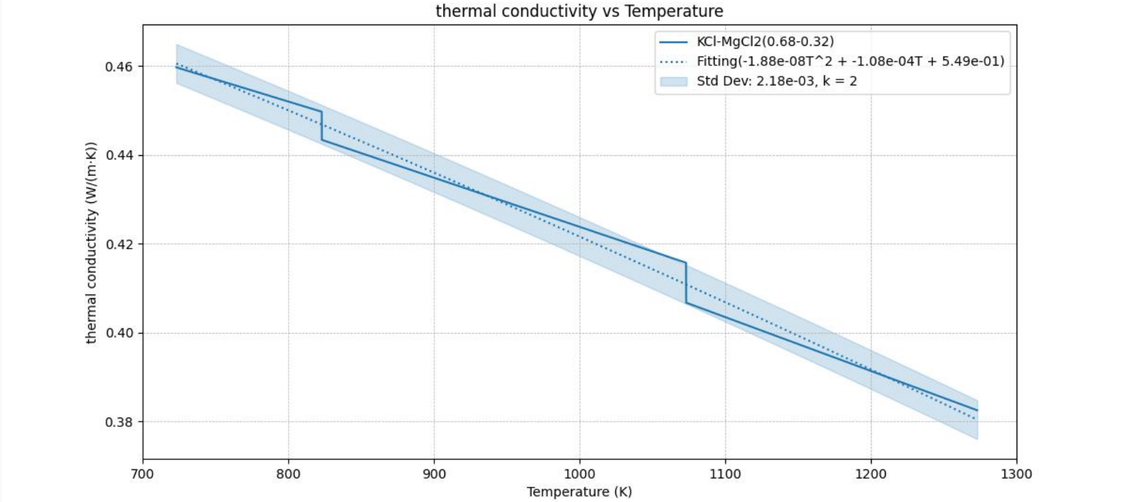
$$UI_{1-\alpha} = [\hat{y} - z_{1-\alpha/2}\, u_{pred}, \hat{y} + z_{1-\alpha/2}\, u_{pred}] \tag{18}$$

APPROXIMATE 95% INTERVAL

$$z_{0.975} = 1.96, UI_{95\%} = [\hat{y} - 1.96\, u_{pred}, \hat{y} + 1.96\, u_{pred}] \tag{19}$$

Stage A — KCl–$MgCl_2$ thermal conductivity at [0.68, 0.32]

Several sources share this composition; the procedure of slides 6 to 10 applies unchanged. Figure shows the pointwise combination, the fitted representative, and the propagated band.



OBSERVATIONS

One curve

Range-edge breaks removed by the continuous fit; fitting term carried into u.

A band, not a number

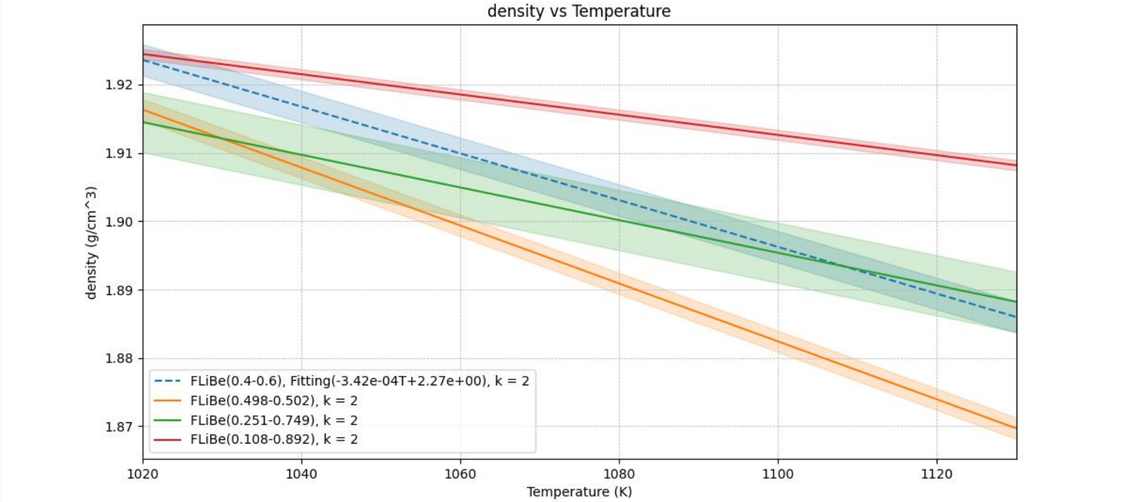
The band widens where sources disagree; that is the least-trusted regime.

An honest answer

No winner is picked; inter-study spread is the visible uncertainty.

Stage B — FLiBe density at [0.4, 0.6]

Stage B runs on an FLiBe composition without direct measurements. Predicted density and neighboring representatives are drawn with the propagated band.



OBSERVATIONS

Weights stop here

Stage A finishes weights; Stage B is geometry only.

Workflow, not validation

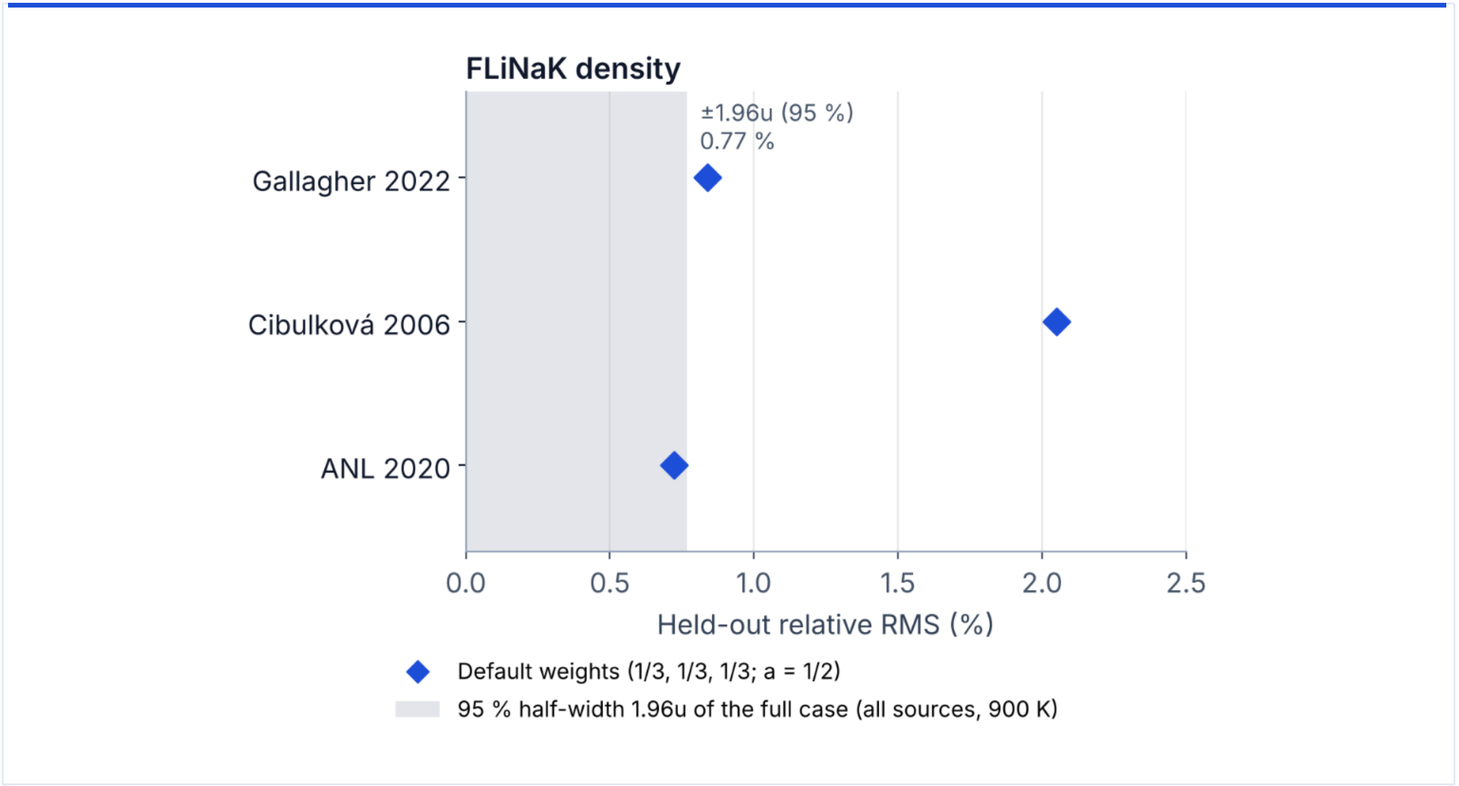
Held-out validation and sensitivity study live in companion documents.

Leave-one-source-out check of the weights

Each source in a three-source group is held out and predicted from the remaining two. Scores, normalization, pointwise weighting and the continuous refit are all recomputed without the held-out source; the prediction is compared with the held-out correlation.

FLiNaK density

HELD-OUT SOURCE	REPORTED ERROR	N
Gallagher 2022	measurement + fit	5
Cibulková 2006	fit only	n/a
ANL 2020	measurement only	18



Some exceed our uncertainty interval - Interstudy errors should be considered in error propagation.(In progress)

Conclusions

C.1

Database

32 source correlations across 4 salts × 4 properties, stored as JSON records with per-source provenance, applicable range, and reported uncertainty.

C.2

Quality weights

3 independent criteria combined into one per-source weight under adjustable coefficients; demonstrations used 1/3 each.

C.3

Two-stage + uncertainty

Representative at a measured composition, interpolation between, standard u propagated through both; leave-one source out revealed a problem.

C.4

Follow-on, openly released

ROM coupling, four transients, salt-by-salt envelope map, open release — residual spread, not choice of weights, sets the remaining uncertainty.

Acknowledgments

FUNDING

This research was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (Project No. RS-2025-02363036).

HOSTS & PARTNER ORGANIZATIONS