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1 Reference density database for 20 aqueous alkali halide solutions

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9 **Abstract:** A reference density database of aqueous alkali halide solutions is presented. The solutes
10 are the 20 alkali halides consisting of the cations, Li⁺, Na⁺, K⁺, Rb⁺, Cs⁺, and anions, F⁻, Cl⁻, Br⁻,
11 I⁻. Experimental density data of these aqueous electrolyte solutions are extensively collected and
12 critically evaluated. A data evaluation procedure is proposed, utilizing support vector regression
13 (SVR) to compare the experimental datasets against each other. Data evaluation is based on
14 agreement with data from other sources rather than accuracy claimed in the literature. Datasets
15 with large deviation from others are identified and removed. The proposed reference database
16 consists of 11081 data points of 586 datasets from 309 references. Maximum deviations between
17 the selected datasets do not exceed 1%, and are smaller than 0.5% for most of the aqueous alkali
18 halide solutions. SVR models are also trained based on the reference database. Data distribution
19 is visualized using a Gaussian mixture model. Applicability domains of the SVR models are
20 analyzed using Williams plots. An executable program is provided for calculations based on the
21 SVR models.

22 **Keywords:** density database, data evaluation, aqueous alkali halide solutions, support vector
23 regression, Gaussian mixture model.

24 Contents

25	1 Introduction.....	2
26	2 Methodology	4
27	2.1 Experimental density data collections.....	4

28	2.2 Data evaluation.....	5
29	2.3 Gaussian mixture model analysis	8
30	2.4 Support vector regression (SVR)	9
31	2.5 Williams plot analysis	12
32	3 Results and discussion	13
33	4 Conclusions.....	17
34	5 Supplementary Material.....	18
35	Acknowledgements.....	18
36	6 Author Declarations	18
37	6.1 Conflict of Interest	18
38	7 Data Availability Statement.....	18
39	8 Reference	18

40 **List of Tables**

41	Table 1. Equations for converting concentration units to ion-based molar fraction.	5
42	Table 2. Reference database for the density of the 20 aqueous alkali halide solutions, and	
43	deviations of the SVR model.	14

44 **List of Figures**

45	Figure 1. Density data evaluation and correlation: (a) workflow and (b) schematics.	7
46	Figure 2. Comparison of collected data (before evaluation) and selected data (after evaluation) of	
47	(water + KCl) density.	8
48	Figure 3. Gaussian mixture model for the density data of the (water + KCl) system.	15
49	Figure 4. Parity plot of the SVR correlation for the density of the (water + KCl) system.	16
50	Figure 5. Williams plot of the SVR correlation for the density data of the (water + KCl) system.	
51		16
52	Figure 6. Example of the user interface for density calculation.	17

53 **1 Introduction**

54 For various industries, accurate measurements and modeling of thermodynamic properties of
55 electrolyte solutions are required ¹. Density is an important property for development of
56 thermodynamic property models ². Furthermore, deriving apparent and partial molal volumes from
57 accurate density data provides insights into the structural information of the aqueous electrolyte
58 solutions ³.

59 In aqueous electrolyte solutions, density is very different from in pure water, being up to 100%
60 larger at high salt composition compared to pure water density at the same temperature and
61 pressure, especially for the heavier salts. In addition, in equations of state, the volumetric
62 parameters are more sensitive to density than to phase equilibria and thermal properties. One
63 should expect large deviations when the density is not included in the objective function ^{4,5}.
64 Therefore, density is an important property that has to be critically evaluated before it can be used
65 in model development.

66 Obtaining a reference database for aqueous alkali halide solutions is important for many
67 reasons. For instance:

- 68 - While density has been extensively measured for some of the aqueous solutions, the
69 measurements are not of the same quality. Critical evaluation of experimental data and
70 removal of data of poor quality are essential steps.
- 71 - The aqueous alkali halide solutions are the first systems that model developers often work
72 on. From the perspective of model development, a reference density database is practical.
- 73 - Many more complicated industrially relevant mixtures consist of water and one or more
74 alkali halides. In the measured data series, usually a few data points are available for
75 aqueous alkali halide solutions. Comparison of the aqueous alkali halide data against a
76 reference database for the system can verify the validity of measurements of the more
77 complicated mixtures before the data are used in industrial applications.

78 In this work, density data of 20 aqueous alkali halide solutions are extensively collected and
79 critically evaluated. Because datasets from hundreds of references are available with very different
80 quality, a fast evaluation approach is proposed here, utilizing the support vector regression (SVR)
81 algorithm to compare the experimental datasets against each other. Datasets that are not consistent
82 with most other datasets are identified and removed. A reference database for the density of
83 aqueous alkali halide solutions is proposed. Based on this reference database, correlations are
84 developed and provided. This work, along with the databases for other properties that were
85 published previously ^{6,7}, can be used for benchmarking future developments of electrolyte equation
86 of state. In addition to this ready-for-use state-of-the-art density database, the proposed data
87 evaluation procedure for density can potentially be used for other properties that do not change
88 drastically in the aqueous phase.

89 **2 Methodology**

90 In this section, the density data collection, evaluation, and correlation procedures are
91 presented. In addition, approaches for assessing the data distribution and model applicability
92 domain are also introduced.

93 **2.1 Experimental density data collections**

94 For the 20 aqueous alkali halide solutions, 14315 density data points of 819 datasets are
95 collected from the CERE aqueous electrolyte databank ⁸ and DETHERM ⁹. Krumgalz et al. ¹⁰
96 presented an evaluated database for densities of a few aqueous electrolyte solutions. 4 of the 20
97 aqueous alkali halide solutions investigated here were covered by their database. Datasets from
98 their database have also been collected along with those from the databanks.

99 In the literature, salt composition was reported in various units. Here the experimental data
100 are converted to the same units for comparisons. Using the equations listed in Table 1,
101 concentration units are converted to ion-based molar fraction, which is usually used in equations
102 of state and activity coefficient models. When the pure water density is needed for the conversion
103 from density difference or apparent molar volume, the reported value from the same reference is
104 used. When pure water density is not provided from the experimental references, it is calculated
105 using IAPWS-95 ^{11,12}. In the cases that pressure was not in reported in the experimental references,
106 it is recorded as 101.325 kPa in this database.

107 Table 1. Equations for converting concentration units to ion-based molar fraction.

Original salt concentration unit	Conversion to ion-based molar fraction ^a
molality	$x_i = Z_i x_i^0 / (Z x_i^0 + 1/M_{\text{water}})$
weight fraction	$x_i = Z_i x_i^0 / M_{\text{salt}} / [Z x_i^0 / M_{\text{salt}} + (1 - x_i^0) / M_{\text{water}}]$
salt-based molar fraction	$x_i = Z_i x_i^0 / [1 + (Z_i - 1)x_i^0]$
molarity	$x_i = Z_i x_i^0 / [Z x_i^0 + (\rho / 1000 - x_i^0 M_{\text{salt}}) / M_{\text{water}}]$
kg salt per kg solvent	$x_i = Z_i x_i^0 / M_{\text{salt}} / (Z x_i^0 / M_{\text{salt}} + 1 / M_{\text{water}})$
mol water per mol salt	$x_i = Z_i / (Z + x_i^0)$
g of salt per 100 cm ³ solution	$x_i = 10 Z_i x_i^0 / M_{\text{salt}} / [10 Z x_i^0 / M_{\text{salt}} + (\rho - 10 x_i^0) / M_{\text{water}}]$

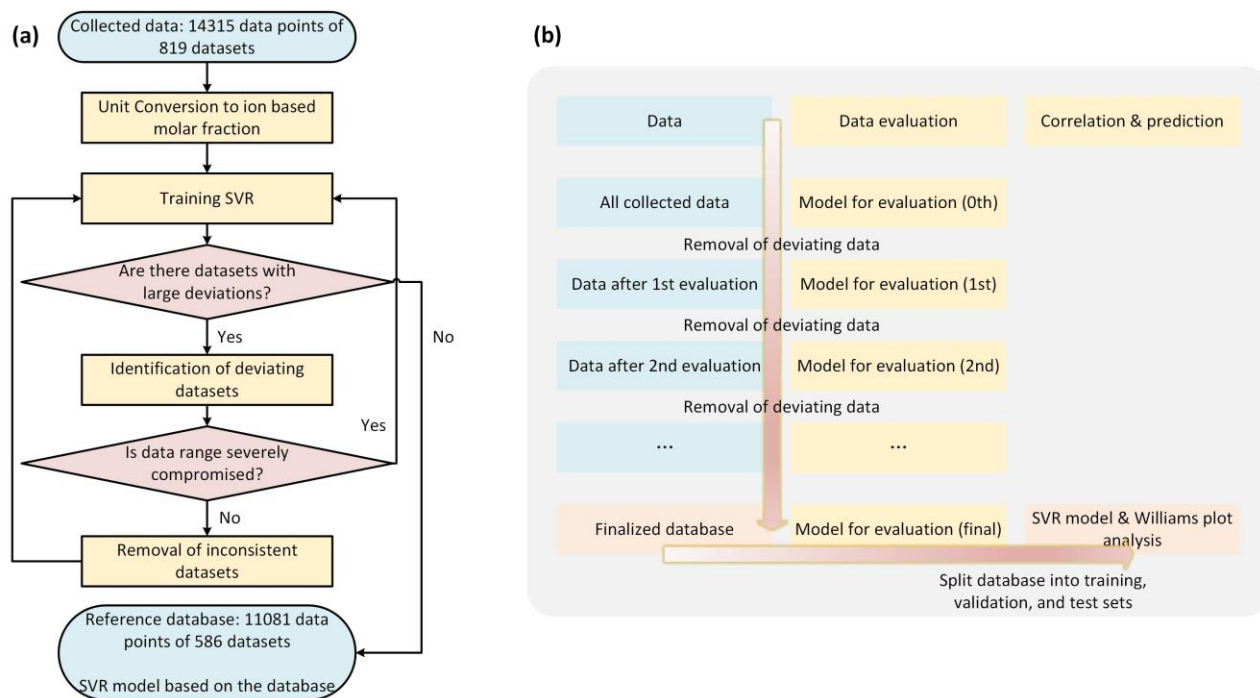
108 a) x_i^0 is the original salt composition unit as noted in the first column of the table. x_i is the ion-based
 109 molar fraction. Z is the total number of ions in the salt, and is 2 for alkali halides. Z_i is the number of ions
 110 i in the salt, and is 1 for alkali halides. M is the molar mass in kg/mol, taken from the NIST Chemistry
 111 WebBook¹³. $M_{\text{water}} = 0.0180153$ kg/mol. ρ is the density of the solution in kg/m³.

112 2.2 Data evaluation

113 The goal of this work is to remove datasets that are outliers, i.e., anomalies, in the collected
 114 databank. Common anomaly detection algorithms include isolation forest, robust covariance,
 115 support vector regression one-class, etc^{14–17}. These classification-based algorithms detect
 116 anomalies based on data distribution. Both response (density) and variables (temperature,
 117 composition, and pressure) are used as inputs for evaluating data distribution. However, in the
 118 scenario of this work, only the data of high accuracy can be selected in the reference database,
 119 while the algorithms are not capable of automatically distinguishing the data points that deviate
 120 from the consistent datasets by only a few percent. More importantly, in these algorithms, the
 121 scarceness of data at high temperature and pressure outweighs the deviations in density, and would
 122 result in undesirable removal of the valuable data in the scarcer region. Therefore, selection of the
 123 reference database can only be achieved based on observation of the deviations of the data points
 124 from a preliminary model that is trained to the data, which reflects deviations of the data points
 125 from each other.

126 The support vector regression (SVR) is used for correlating the collected data and for
 127 comparing the data with each other. Through the Gibbs phase rule, it is known that a homogeneous
 128 mixture of water and a salt has 3 degrees of freedom, i.e., composition (x), temperature (T), and
 129 pressure (p). This is different from in the usual applications of the machine learning models on

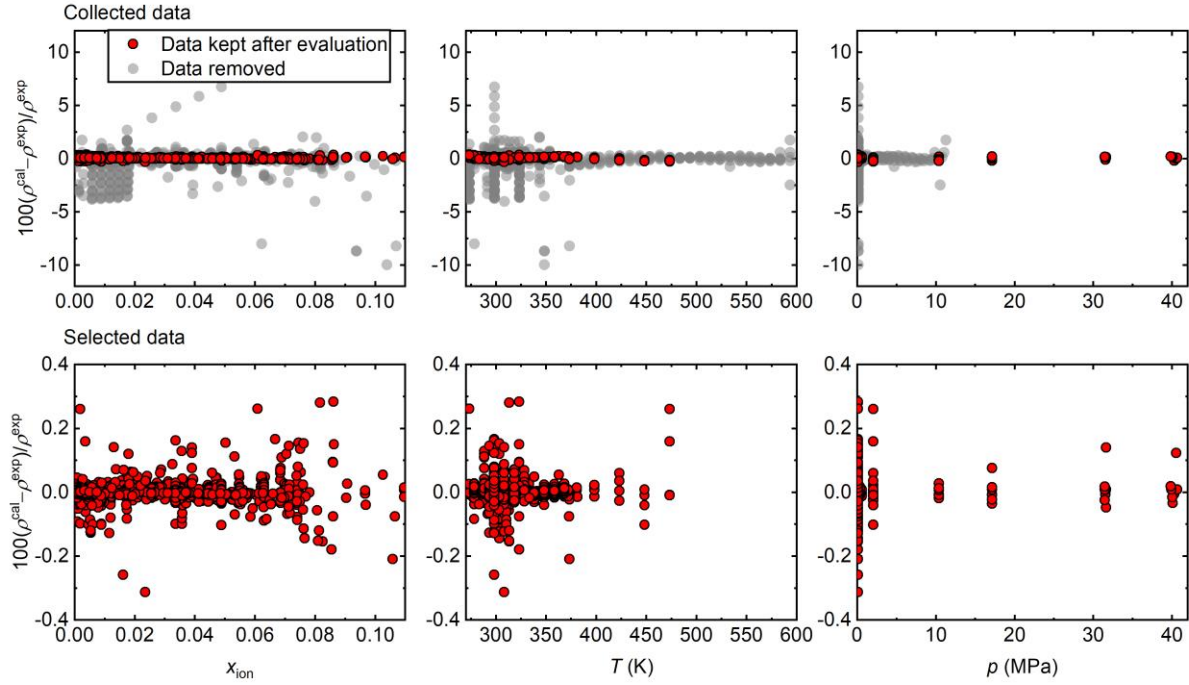
130 predicting thermodynamic properties (e.g., group contribution and quantitative structure-property
131 relationship models (QSPR)¹⁸⁻²⁰), in which case dominant features have to be selected and do not
132 contain complete information of the response. Therefore, given datasets that are consistent with
133 each other, the experimental data should be regressed to the SVR model with very high accuracy.
134 The accuracy indicates agreement between the experimental datasets in addition to agreement of
135 the datasets with the trained model. On the other hand, when a dataset deviates much from the
136 trained SVR model in a region where other experimental datasets agree well with the model, we
137 can conclude that the deviating dataset is inconsistent with the other experimental datasets. Plotted
138 against the 3 degrees of freedom, it can be observed whether a data point is “deviating” beyond
139 the scattering of other data; it can also be observed whether the data range is severely compromised
140 when a dataset is removed as deviations are observed to be larger compared to the other datasets.
141 When a data point from a dataset is considered to be deviating too much from the other data, the
142 entire dataset that contains the deviating data point is removed. The procedure is repeated until all
143 datasets agree well with each other up to a desirable accuracy without the need to remove any more
144 experimental datasets. In general, no more than 4 regressions were needed. In the evaluation, all
145 the data are included for regressing the SVR model, because the regressed model is intended only
146 for comparing the datasets against each other, rather than for calculations. After the reference
147 database is finalized, it is split into training, validation, and test sets for correlating SVR models
148 that are used for calculations, as will be explained in Section 2.4. Figure 1 summarizes the
149 procedure of density data evaluation and correlation. The evaluation procedure is applied for the
150 20 aqueous alkali halide solutions. Then, the reference database is finalized, and is used for training
151 the SVR models.



152

153 Figure 1. Density data evaluation and correlation: (a) workflow and (b) schematics.

154 Figure 2 shows a comparison of the collected data and selected data (reference database) of
 155 the (water + KCl) density as an example of the evaluation procedure. At the start, input data include
 156 some datasets that deviate from others by more than 10%, and some datasets that already deviate
 157 from others by only 1~3%, but fall in the range that other datasets agree very well with each other.
 158 As these datasets are removed, agreement between the remaining datasets is improved. For this
 159 case, the procedure took 3 rounds of evaluations. The data that have been excluded in the final
 160 reference database are marked as grey in the graphs of the collected data to show the comparably
 161 larger deviations compared to the data that have been kept. In the graphs on the second row, only
 162 the kept data are shown, with a much smaller scale of deviation. Before the evaluation, the
 163 collected data present deviations of more than 15% in some cases, and much scattering in regions
 164 with a lot of data. At the end, all the remaining data agree with each other within 0.5%. The
 165 procedure is performed on the density data of the 20 aqueous alkali halide solutions.



166

167 Figure 2. Comparison of collected data (before evaluation) and selected data (after evaluation) of (water +
 168 KCl) density. Data that are removed in the finalized reference database are marked as grey in the graphs
 169 of the collected data.

170 2.3 Gaussian mixture model analysis

171 The Gaussian mixture model (GMM) is a probability model that implements iterative
 172 expectation maximization algorithm for analyzing data clustering²¹. In this work, it is used for
 173 providing a qualitative visualization of data distribution. GMMs are trained for the selected density
 174 data of each aqueous alkali halide solution. The GMM is defined as:

$$q(\mathbf{z}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{k=1}^K \pi_k \mathcal{N}(\mathbf{z}|\mu_k, \Sigma_k) \quad (1)$$

$$\sum_{k=1}^K \pi_k = 1 \quad (2)$$

175 where q is the likelihood (usually denoted as p , but noted as q here to avoid confusion with the
 176 pressure), $\mathbf{z} = (T, p, x)$ is the input (each data point), $\boldsymbol{\pi} = \{\pi_1, \dots, \pi_K\}$ are mixing coefficients, and
 177 $\boldsymbol{\mu} = \{\mu_1, \dots, \mu_K\}$ and $\boldsymbol{\Sigma} = \{\Sigma_1, \dots, \Sigma_K\}$ specify the mean and covariance of each Gaussian
 178 component $\mathcal{N}(\mathbf{z}|\mu_k, \Sigma_k)$, respectively, k denotes the k th GMM component, K denotes the total

179 number of GMM components, and \mathcal{N} denotes the Gaussian distribution. $\boldsymbol{\pi}$, $\boldsymbol{\mu}$, and $\boldsymbol{\Sigma}$ are
 180 parameters that are trained in the GMM to approximate the data distribution, \mathbf{z} . Given a training
 181 set, the parameters $\boldsymbol{\pi}$, $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ are first initialized via the k-means++ algorithm ²² and then
 182 estimated through the iterative Expectation-Maximization (EM) algorithm to maximize the
 183 likelihood ²³, according to:

$$\ln q(\mathbf{Z}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{n=1}^N \ln \sum_{k=1}^K \pi_k \mathcal{N}(\mathbf{z}_n | \mu_k, \Sigma_k) \quad (3)$$

184 where $\mathbf{Z} = (\mathbf{T}, \mathbf{p}, \mathbf{x})$ is the input matrix, N is the number of data points, and \mathbf{z}_n is for the n th data
 185 point. In addition, to avoid overfitting, K is selected to minimize Bayesian information criterion
 186 (BIC) ²⁴, which is defined as $\text{BIC} = \ln(N) M - 2 \ln(\hat{L})$, where N is the number of data points, M
 187 represents the number of estimated parameters, and \hat{L} denotes the maximized value of the
 188 likelihood function of the model.

189 GMM can provide a qualitative visualization of data distribution using a contour plot. In
 190 addition, its convergence also reflects to some extent the quality of our collected database.
 191 Furthermore, in this work, we also use the GMM to determine if calculated data points can be
 192 regarded as within the range of the database. The procedure is known as novelty detection ²⁵. Any
 193 data point located in a low data-distribution-density region can be considered a novelty. In this
 194 way, GMM enables us to determine whether our database can be applied to a new condition. An
 195 executable program is provided in the Supplementary Material for calculations. The GMM plot of
 196 the database is presented in the user interface as calculations are made. In this way, whether the
 197 calculations are within the ranges of the proposed database is visualized.

198 **2.4 Support vector regression (SVR)**

199 SVR provides the flexibility to define how much error is acceptable in the regression ²⁶.
 200 Deviations below a threshold, ε , are considered unimportant. In this way, a tube is defined of which
 201 the centerline is the prediction of the SVR model. Within the tube, deviations are not penalized in
 202 the objective function. The very idea of SVR is suitable for identifying datasets that present larger
 203 deviations compared to others. Advantages of SVR include that its generalization capability and
 204 prediction accuracy are excellent ²⁷. Therefore, SVR is very suitable for evaluating and correlating

205 data of thermodynamic properties, for which extensive measurements are prohibitively expensive,
 206 and evenly distributed data are usually unavailable.

207 In SVR, Eq. (5) is minimized subject to the constraints of Eq. (6).

$$\frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^N (\xi_i + \xi_i^*) \quad (5)$$

$$y_i - \mathbf{w}^T \cdot \phi(\mathbf{x}_i) - b \leq \varepsilon - \xi_i, \forall i = 1, \dots, N \quad (6a)$$

$$\mathbf{w}^T \cdot \phi(\mathbf{x}_i) + b - y_i \leq \varepsilon + \xi_i^*, \forall i = 1, \dots, N \quad (6b)$$

$$\xi_i \geq 0, \forall i = 1, \dots, N \quad (6c)$$

$$\xi_i^* \geq 0, \forall i = 1, \dots, N \quad (6d)$$

208 where \mathbf{w} is the coefficient factor, C is the box constraint, ε is the margin within which errors are
 209 ignored, ξ_i and ξ_i^* are the slack variables, y_i is the response, \mathbf{x}_i is the variable vector, ϕ and b are
 210 defined in the SVR approximation:

$$f(\mathbf{x}) = \mathbf{w}^T \cdot \phi(\mathbf{x}) + b \quad (7)$$

211 The slack variables, ξ_i and ξ_i^* , are introduced for each data point, and allow regression errors
 212 to be larger than the margin error value, ε .

213 Eqs. (5) and (6) are transformed into the dual formula using the Lagrange multipliers²⁸, α_i
 214 and α_i^* .

$$L(\alpha) = \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N (\alpha_i - \alpha_i^*)(\alpha_j - \alpha_j^*) K(\mathbf{x}_i, \mathbf{x}_j) + \varepsilon \sum_{i=1}^N (\alpha_i + \alpha_i^*) - \sum_{i=1}^N y_i (\alpha_i - \alpha_i^*) \quad (8)$$

$$\sum_{i=1}^N (\alpha_i - \alpha_i^*) = 0, \forall i = 1, \dots, N \quad (9a)$$

$$0 \leq \alpha_i \leq C, \forall i = 1, \dots, N \quad (9b)$$

$$0 \leq \alpha_i^* \leq C, \forall i = 1, \dots, N \quad (9c)$$

215 Instead of Eq. (5), Eq. (8) is minimized subject the constraints of Eq. (9).

216 In this work, the Gaussian kernel function ²⁹ is used:

$$K(\mathbf{x}_i, \mathbf{x}_j) \equiv \phi(\mathbf{x}_i) \cdot \phi(\mathbf{x}_j) = \exp\left(-\|\mathbf{x}_i - \mathbf{x}_j\|^2\right) \quad (10)$$

217 Predictions of a response at given x is calculated according to,

$$f(\mathbf{x}) = \sum_{i=1}^N (\alpha_i - \alpha_i^*) K(\mathbf{x}_i, \mathbf{x}) + b \quad (11)$$

218 The data are standardized before the model is trained. The SVR implementation in Matlab is
219 used. The training process of the SVR model is performed in nested loops:

- 220 - In the outer loop, the SVR hyper parameters, i.e., the box constraint, kernel scale, and
221 threshold, ε , are optimized using the Bayesian optimization ³⁰⁻³² with the expected-
222 improvement-plus algorithm ³⁰ as the acquisition function to choose the next promising
223 hyper parameter set, which is expected to have smaller errors for the validation set.
- 224 - In the inner loop, with fixed hyper parameters, the SVR model is optimized using the
225 sequential minimal optimization algorithm ³³.

226 In practice, the maximum number of iterations is set at 100, which turned out to be large enough
227 for convergence.

228 The SVR model is used in both the evaluation and correlation of the database. In the
229 evaluation, the entire database is used for training the SVR model in each step, as shown in Figure
230 1b.

231 In the correlation, the obtained reference database is split into training, validation, and test
232 sets. For each solution, 20% of the data are set aside as test sets; the remaining 80% of the data are
233 used as training/validation sets. 10-fold cross-validation is implemented for training the SVR
234 models. The accuracy of the model on the training/validation and test sets are investigated. An

235 executable program with user interface are provided in the Supplementary Material for
236 calculations using the trained model.

237 **2.5 Williams plot analysis**

238 In addition to the GMM analysis, the Williams plot analysis³⁴ is employed for visualizing
239 distribution of the selected data.

$$h_i = \mathbf{x}_i^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}_i \quad (12)$$

240 where h_i is the hat value, \mathbf{x}_i is the variable vector of a data point, and \mathbf{X} is the variable matrix of
241 the entire database. The threshold value $h^* = 3(P + 1)/N$ is also calculated and compared with
242 the hat value of all the data points, where $P = 3$ is the number of variables, and N is the number
243 of data points.

244 In the Williams plot, the relative deviation of the SVR model is plotted against the hat value.
245 The approach is widely used for evaluating the applicability domain in QSAR models. When $h_i >$
246 h^* , in QSAR models, the calculation is considered extrapolated and could be less reliable; however,
247 for the density correlation here, the data point is considered to be located in a scarcer region.
248 Because of the completeness of information in thermodynamic (3 degrees of freedom of the
249 density of the mixture of water and a salt) as compared to the incompleteness of information for
250 mapping between molecular structure and activity (as in QSAR models), the threshold can be
251 considered much stricter here than in QSAR models. As will be discussed in Section 3 and in the
252 Supplementary Material, deviations do not significantly increase beyond the threshold, indicating
253 good correlation of the model in scarcer regions. Therefore, this threshold hat value of the database
254 is not intended as a strict bar beyond which calculation should be prohibited. Instead, the threshold
255 serves as merely an indicator that the calculations are made in scarcer regions.

256 Furthermore, when calculations are made using the correlation, comparing the hat value of
257 the calculations with the threshold and with the hat values of data points in the database visualizes
258 whether the calculated data are located in a region where there are extensive data points that have
259 been used in training the correlation.

260 **3 Results and discussion**

261 The collected datasets are evaluated using the procedure explained in Section 2. Table 2
262 provides the resulting reference database for the density of the 20 aqueous alkali halide solutions.
263 11081 data points of 586 datasets from 309 references are included in the database. The references
264 are provided in the last column of the table. We recommend that these references be cited when
265 using the database. The database is provided in the Supplementary Material. As an example, the
266 (water + KCl) system is discussed in detail here. The plots for the other aqueous alkali halide
267 solutions are provided in the Supplementary Material. Figure 3 shows the GMM plot for the
268 density data of the (water + KCl) system. The contour is to visualize data distribution. The GMM
269 is analyzed on the T - x_{ion} projection, because most of the density data of the system are distributed
270 at or near atmospheric pressure. The experimental data are plotted together with the contours.

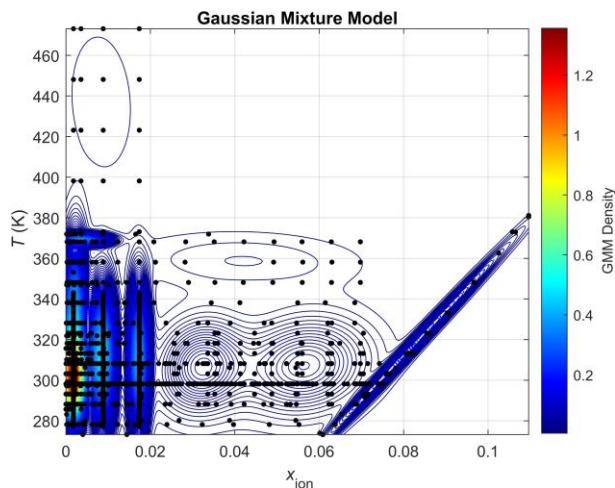
71

72

Table 2. Reference database for the density of the 20 aqueous alkali halide solutions, and deviations of the SVR model. AAD is the percentage average absolute deviation. MAD is the percentage maximum absolute deviation.

Water +	Collected data		Selected data		T (K)	x_{ion}	Reference	AAD (%)		MAD (%)	
	No. of data points	No. of datasets	No. of data points	No. of datasets				Training- Validation	Test	Training- Validation	Test
LiF	55	5	55	5	291.15-308.15	0-0.0019	35-39	0.0031	0.0014	0.12	0.0030
NaF	347	17	347	17	273.15-572.70	0-0.019	36-52	0.013	0.031	0.59	0.60
KF	465	18	448	14	293.15-572.70	0-0.17	36,37,42-47,53-58	0.055	0.050	0.53	0.74
RbF	32	4	32	4	291.15-333.15	0-0.067	36,42,43,59	0.057	0.084	0.42	0.37
CsF	27	3	27	3	293.15-333.15	0-0.050	36,42,43	0.15	0.13	0.42	0.27
LiCl	1650	77	1181	57	273.15-549.80	0-0.27	36,41-44,60-111	0.031	0.024	0.57	0.57
NaCl	3647	185	2687	137	253.00-573.35	0-0.098	41-44,48,54,93-223	0.018	0.012	0.25	0.16
KCl	2264	160	1624	105	273.15-473.15	0-0.11	40,41,43-45,53,54,91,92,99-111,196-217,223-284	0.017	0.012	0.31	0.30
RbCl	301	30	168	14	288.15-328.15	0-0.12	41,43,44,52,54,101-104,123,223,281,282,285	0.064	0.10	0.34	0.36
CsCl	408	36	351	30	273.85-473.15	0-0.19	42,43,88,91,102-107,119-124,196,217,223,282,285-294	0.20	0.29	1.0	0.75
LiBr	939	25	698	19	229.15-525.00	0-0.22	36,42,43,66-68,97,108,109,137,285,295-302	0.045	0.062	0.41	0.51
NaBr	1319	55	1204	37	273.15-549.80	0-0.14	36,42-44,62,66,73,97,108-110,195,217,223-225,282,285-287,302-317	0.055	0.040	1.0	0.39
KBr	1083	67	856	49	270.91-473.15	0-0.12	36,41-44,56,62,66,96,100,102,108,109,135-138,213-217,221,224,229-236,282,285,290,295,302,314,315,318-327	0.037	0.030	0.49	0.20
RbBr	77	6	38	4	291.15-333.15	0-0.074	36,42,43,52	0.082	0.048	0.41	0.070
CsBr	120	12	50	7	298.15-308.15	0-0.073	36,43,62,88,223,286,287	0.12	0.18	0.43	0.28
LiI	352	17	289	10	278.15-575.75	0-0.12	42,62,68,97,107,109,285,328-330	0.056	0.051	0.84	0.19
NaI	271	38	165	20	293.15-323.15	0-0.15	36,43,44,54,97,102,107-109,154,237,290,298,311,331-336	0.095	0.085	1.7	0.15
KI	750	46	661	37	270.32-473.15	0-0.13	36,41,43-45,48,53,56,93,100,107-109,154,212-216,235-238,282,285,290,295,305,318,322,336-342	0.022	0.033	0.45	0.63
RbI	64	7	56	6	273.15-333.15	0-0.11	36,42,43,52,107,137	0.21	0.28	0.87	0.38
CsI	144	11	144	11	273.15-343.34	0-0.058	35,36,42,43,107,137,223,286,287,290,343	0.093	0.13	0.46	0.38

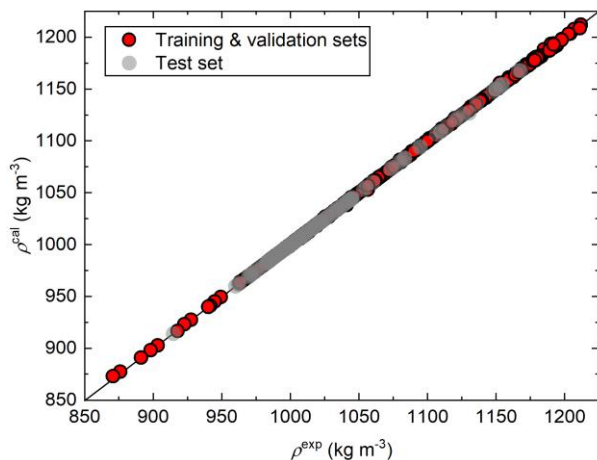
73



274

275 Figure 3. Gaussian mixture model for the density data of the (water + KCl) system. The contour plot is the
 276 calculated data-distribution-density. The dots are data points of the database.

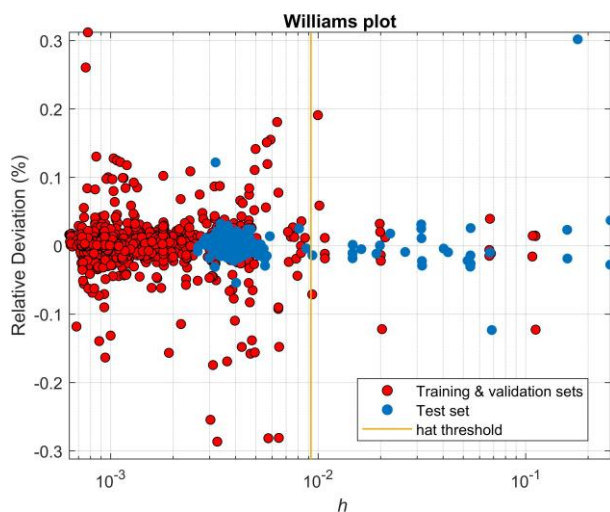
277 Based on the database, an SVR model is developed according to the procedure introduced in
 278 Section 2.4. Figure 4 shows the parity plot of the SVR correlation for the density of the (water +
 279 KCl) system. The test set is calculated with comparable accuracy compared to the training and
 280 validation sets. The SVR model is very accurate within the range of the database. Percentage
 281 average absolute deviation (AAD) and percentage maximum absolute deviation (MAD) for the 20
 282 aqueous alkali halide solutions are provided in Table 2. The deviations are slightly larger compared
 283 to the maximum deviations in the data evaluation step, in which the models are trained on all the
 284 data of the aqueous alkali halide solutions (maximum deviations between the selected datasets do
 285 not exceed 1.1%, and are smaller than 0.5% for most of the aqueous alkali halide solutions). We
 286 expect that training the SVR model based on the entire database would slightly improve correlation
 287 accuracy without hampering the extrapolation performance of the model. However, we would not
 288 be able to verify this without any data for the test set. Therefore, 20% of the database is set aside
 289 as a test set.



290

291 Figure 4. Parity plot of the SVR correlation for the density of the (water + KCl) system.

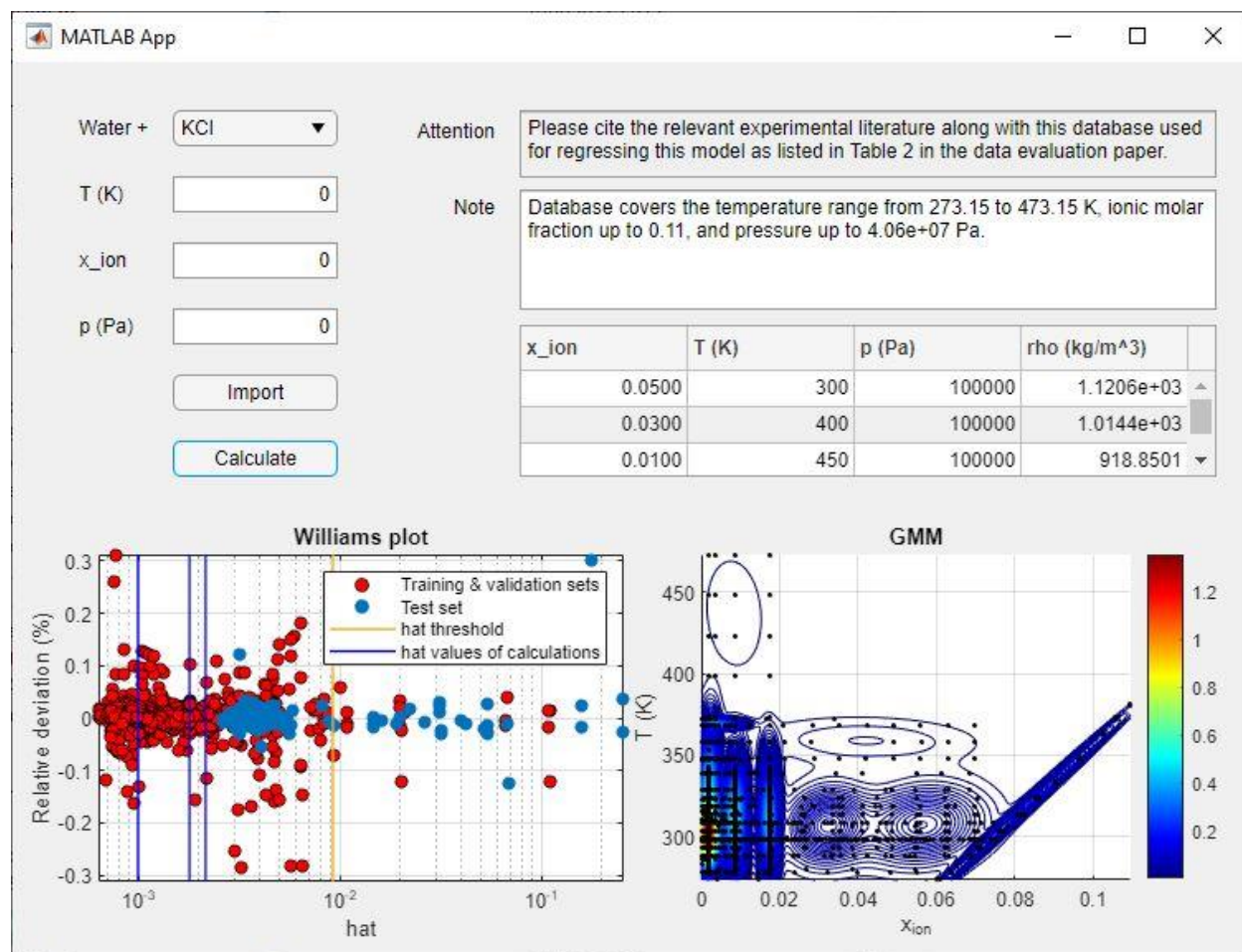
292 Figure 5 shows the Williams plot of the SVR correlation for the density data of the (water +
 293 KCl) system. There are some data points that exceed the threshold hat value. Most of these data
 294 points are at high pressure, while the majority in the database are at atmospheric pressure. However,
 295 deviations are not larger compared to the data points below the threshold. For the test set, the
 296 deviations are comparable to those of the training and validation sets. The good correlation and
 297 prediction show that the database is reliable on the edges of the data coverage, where there are
 298 much fewer data points, and that the SVR model is not over fitted. The Williams plot for the SVR
 299 model of the other aqueous alkali halide solutions are provided in the Supplementary Material.
 300 The behavior is similar to that of the (water + KCl) system.



301

302 Figure 5. Williams plot of the SVR correlation for the density data of the (water + KCl) system. The hat
 303 values are calculated using Eq. (13) for the training & validation sets, and for the test set.

304 An executable program is provided in the Supplementary Material for calculating density of
 305 the aqueous alkali halide solutions. Figure 6 shows an example of the user interface. Density results
 306 are provided along with data ranges of the solution, and illustrations of the calculations plotted on
 307 the Williams and GMM plots.



308
 309 Figure 6. Example of the user interface for density calculation. The salt is selected using the dropdown
 310 list on the top-left corner. Then, input can be made in the numeric edit fields, or imported from a file. A
 311 sample file is provided in the Supplementary Material. Then, at the click of the “Calculate” button, results
 312 are shown in the table on the right side. Notes about the calculation are displayed above the table,
 313 summarizing ranges of the database for the mixture, or, in the case of a calculation beyond the database
 314 ranges, warnings about which input variable exceeds the range. The Williams and GMM plots are shown
 315 on the bottom.

316 4 Conclusions

317 In this work, the experimental density data of 20 aqueous alkali halide solutions are
 318 extensively collected and critically evaluated using machine learning. A reference database

319 consisting of 11081 data points of 586 datasets from 309 references is constructed. Maximum
320 deviations between the selected datasets do not exceed 1.1%, and are smaller than 0.5% for most
321 of the aqueous alkali halide solutions. Data distribution is visualized using the Williams plot and
322 Gaussian mixture model. Support vector regression models are developed based on the database,
323 and implemented in an executable program.

324 The obtained database and models can be utilized in the development of electrolyte equations
325 of state. The proposed data evaluation procedure for density can potentially be used for other
326 properties that do not change drastically in the aqueous phase.

327 **5 Supplementary Material**

328 The followings are provided in the Supplementary Material:

- 329 - An Excel file containing all the data.
- 330 - An executable program for density calculation.
- 331 - GMM and Williams plots for the aqueous alkali halide solutions.

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336 **6 Author Declarations**

337 **6.1 Conflict of Interest**

338 The authors declare no competing financial interest.

339 **7 Data Availability Statement**

340 The data that support the findings of this study are available within the article and its
341 supplementary material.

342 **8 Reference**

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