




Reference Density Database for 20 Aqueous Alkali Halide Solutions

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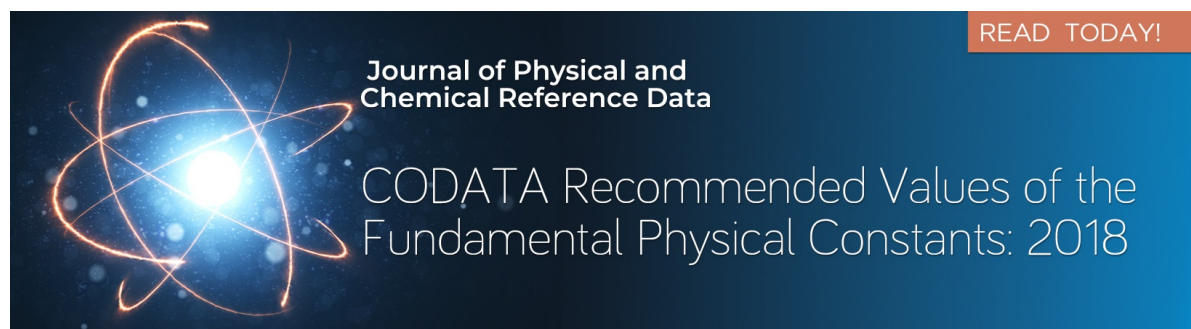
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ABSTRACT

A reference density database of aqueous alkali halide solutions is presented. The solutes are the 20 alkali halides consisting of the cations Li^+ , Na^+ , K^+ , Rb^+ , Cs^+ , and anions F^- , Cl^- , Br^- , I^- . Experimental density data of these aqueous electrolyte solutions are extensively collected and critically evaluated. A data evaluation procedure is proposed, utilizing support vector regression (SVR) to compare the experimental datasets against each other. Data evaluation is based on agreement with data from other sources rather than accuracy claimed in the literature. Datasets with large deviation from others are identified and removed. The proposed reference database consists of 11 081 data points of 586 datasets from 309 references. Maximum deviations between the selected datasets do not exceed 1%, and are smaller than 0.5% for most of the aqueous alkali halide solutions. SVR models are also trained based on the reference database. Data distribution is visualized using a Gaussian mixture model. Applicability domains of the SVR models are analyzed using Williams plots. An executable program is provided for calculations based on the SVR models.

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Key words: aqueous alkali halide solutions; density database; data evaluation; Gaussian mixture model; support vector regression.

CONTENTS

1. Introduction	2
2. Methodology	2
2.1. Experimental density data collections	2
2.2. Data evaluation	3
2.3. Gaussian mixture model analysis	3
2.4. Support vector regression (SVR)	5
2.5. Williams plot analysis	5
3. Results and Discussion	7
4. Conclusions	8
5. Supplementary Material	9
Acknowledgments	9
6. Author Declarations	9
6.1. Conflict of Interest	9
7. Data Availability	9
8. References	9

List of Tables

1. Equations for converting concentration units to ion-based molar fraction	2
2. Reference database for the density of the 20 aqueous alkali halide solutions, and deviations of the SVR model.	6

List of Figures

1. Density data evaluation and correlation: (a) workflow and (b) schematics.	4
2. Comparison of collected data (before evaluation) and selected data (after evaluation) of (water + KCl) density.	4
3. Gaussian mixture model for the density data of the (water + KCl) system.	7
4. Parity plot of the SVR correlation for the density of the (water + KCl) system.	7
5. Williams plot of the SVR correlation for the density data of the (water + KCl) system.	8
6. Example of the user interface for density calculation.	8

1. Introduction

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

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

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

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

In this work, density data of 20 aqueous alkali halide solutions are extensively collected and critically evaluated. Because datasets from hundreds of references are available with very different quality, a fast evaluation approach is proposed here, utilizing the support vector regression (SVR) algorithm to compare the experimental

datasets against each other. Datasets that are not consistent with most other datasets are identified and removed. A reference database for the density of aqueous alkali halide solutions is proposed. Based on this reference database, correlations are developed and provided. This work, along with the databases for other properties that were published previously,^{6,7} can be used for benchmarking future developments of electrolyte equations of state. In addition to this ready-for-use state-of-the-art density database, the proposed data evaluation procedure for density can potentially be used for other properties that do not change drastically in the aqueous phase.

2. Methodology

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

2.1. Experimental density data collections

For the 20 aqueous alkali halide solutions, 14 315 density data points of 819 datasets are collected from the CERE aqueous electrolyte databank⁸ and DETHERM.⁹ Krumgalz *et al.*¹⁰ presented an evaluated database for densities of a few aqueous electrolyte solutions. Four of the 20 aqueous alkali halide solutions investigated here were covered by their database. Datasets from their database have also been collected along with those from the databanks.

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

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	$x_i = Z_i x_i^0 / [1 + (Z - 1)x_i^0]$
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	$x_i = 10 Z_i x_i^0 / M_{\text{salt}} / [10 Z x_i^0 / M_{\text{salt}} + (\rho - 10 x_i^0) / M_{\text{water}}]$

^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 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 i in the salt and is 1 for alkali halides. M is the molar mass in kg/mol, taken from the NIST Chemistry WebBook.¹³ $M_{\text{water}} = 0.018\,015\,3$ kg/mol. ρ is the density of the solution in kg/m³.

2.2. Data evaluation

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

SVR is used for correlating the collected data and for comparing the data with each other. Through the Gibbs phase rule, it is known that a homogeneous mixture of water and a salt has three degrees of freedom, i.e., composition (x), temperature (T), and pressure (p). This is different from in the usual applications of the machine learning models on predicting thermodynamic properties [e.g., group contribution and quantitative structure–property relationship models (QSPR)^{18–20}], in which case dominant features have to be selected and do not contain complete information of the response. Therefore, given datasets that are consistent with each other, the experimental data should be regressed to the SVR model with very high accuracy. The accuracy indicates agreement between the experimental datasets in addition to agreement of the datasets with the trained model. On the other hand, when a dataset deviates much from the trained SVR model in a region where other experimental datasets agree well with the model, we can conclude that the deviating dataset is inconsistent with the other experimental datasets. Plotted against the three degrees of freedom, it can be observed whether a data point is “deviating” beyond the scatter of other data; it can also be observed whether the data range is severely compromised when a dataset is removed as deviations are observed to be larger compared to the other datasets. When a data point from a dataset is considered to be deviating too much from the other data, the entire dataset that contains the deviating data point is removed. The procedure is repeated until all datasets agree well with each other up to a desirable accuracy without the need to remove any more experimental datasets. In general, no more than four regressions were needed. In the evaluation, all the data are included for regressing the SVR model because the regressed model is intended only for comparing the datasets against each other, rather than for calculations. After the reference database is finalized, it is split into training, validation, and test sets for correlating SVR models that are used for calculations, as will be explained in Sec. 2.4. Figure 1 summarizes the procedure of density data evaluation and correlation. The evaluation procedure is applied for the 20 aqueous alkali halide solutions. Then, the reference database is finalized and is used for training the SVR models.

Figure 2 shows a comparison of the collected data and selected data (reference database) of the (water + KCl) density as an example of the evaluation procedure. At the start, input data include some datasets that deviate from others by more than 10%, and some datasets that, although they deviate from others by only 1%–3%, fall in the range where other datasets agree very well with each other. As these datasets are removed, the agreement between the remaining datasets is improved. For this case, the procedure took three rounds of evaluations. The data that were excluded in the final reference database are marked as gray in the graphs of the collected data to show the comparably larger deviations compared to the data that have been kept. In the graphs on the second row, only the kept data are shown, with a much smaller scale of deviation. Before the evaluation, the collected data present deviations of more than 10% in some cases, and much scattering in regions with a lot of data. At the end, all the remaining data agree with each other within 0.4%. The procedure is performed on the density data of the 20 aqueous alkali halide solutions.

2.3. Gaussian mixture model analysis

The Gaussian mixture model (GMM) is a probability model that implements iterative expectation maximization algorithm for analyzing data clustering.²¹ In this work, it is used for providing a qualitative visualization of data distribution. GMMs are trained for the selected density data of each aqueous alkali halide solution. The GMM is defined as

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

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

where q is the likelihood (usually denoted as p , but noted as q here to avoid confusion with the pressure), $\mathbf{z} = (T, p, x)$ is the input (each data point), $\boldsymbol{\pi} = \{\pi_1, \dots, \pi_K\}$ are mixing coefficients, and $\boldsymbol{\mu} = \{\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_K\}$ and $\boldsymbol{\Sigma} = \{\boldsymbol{\Sigma}_1, \dots, \boldsymbol{\Sigma}_K\}$ specify the mean and covariance of each Gaussian component $\mathcal{N}(\mathbf{z}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$, respectively, k denotes the k th GMM component, K denotes the total number of GMM components, and \mathcal{N} denotes the Gaussian distribution. $\boldsymbol{\pi}$, $\boldsymbol{\mu}$, and $\boldsymbol{\Sigma}$ are parameters that are trained in the GMM to approximate the data distribution, \mathbf{z} . Given a training set, the parameters $\boldsymbol{\pi}$, $\boldsymbol{\mu}$, and $\boldsymbol{\Sigma}$ are first initialized via the k-means++ algorithm²² and then estimated through the iterative Expectation-Maximization (EM) algorithm to maximize the likelihood,²³ according to

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

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

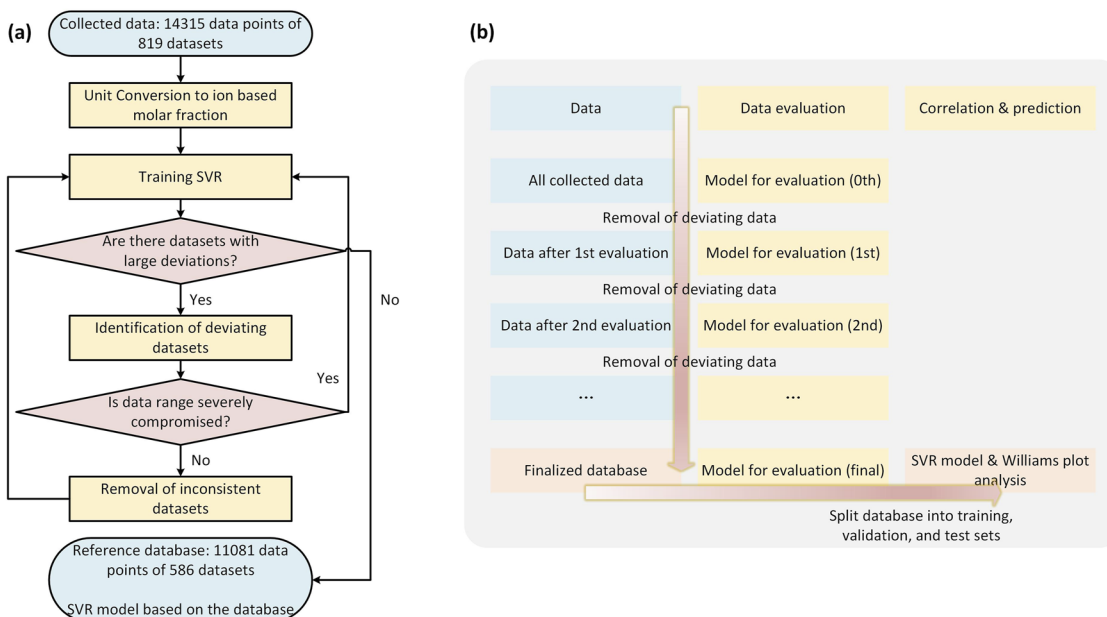


FIG. 1. Density data evaluation and correlation: (a) workflow and (b) schematics.

GMM can provide a qualitative visualization of data distribution using a contour plot. In addition, its convergence also reflects to some extent the quality of our collected database. Furthermore, in this work, we also use the GMM to determine if calculated data

points can be regarded as within the range of the database. The procedure is known as novelty detection.²⁵ Any data point located in a low data-distribution-density region can be considered a novelty. In this way, GMM enables us to determine whether our database can

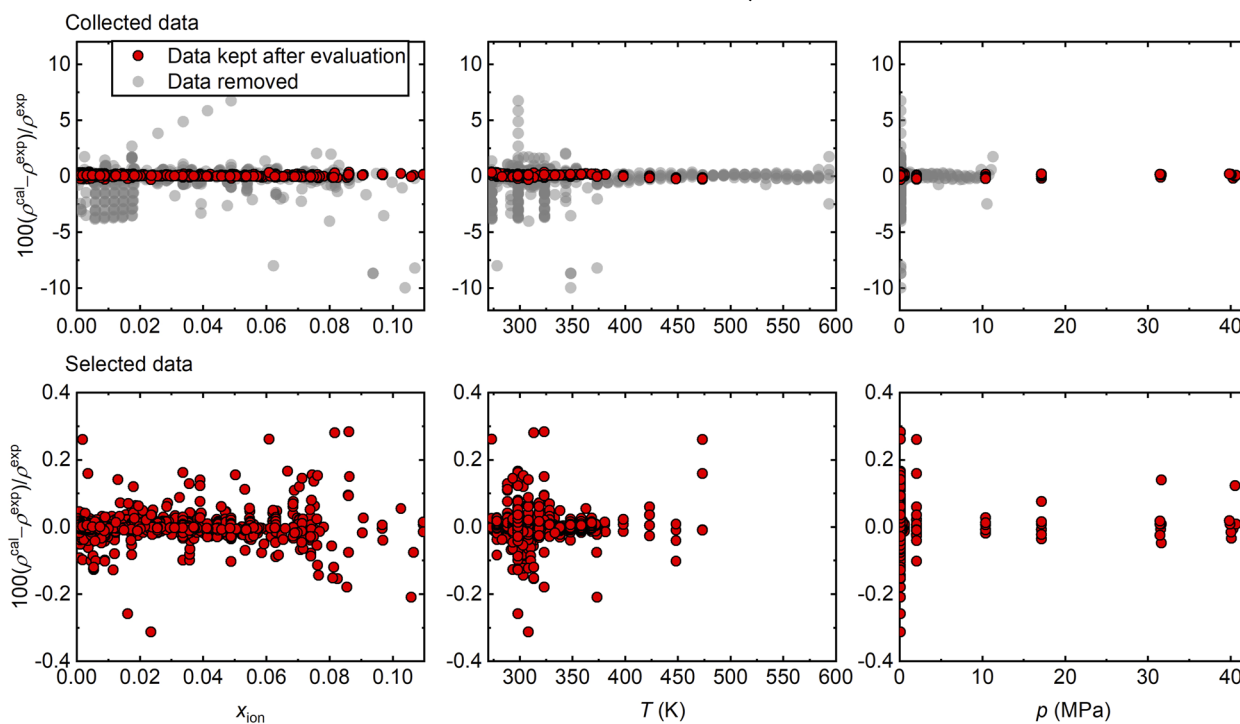


FIG. 2. Comparison of collected data (before evaluation) and selected data (after evaluation) of (water + KCl) density. Data that are removed in the finalized reference database are marked as gray in the graphs of the collected data.

be applied to a new condition. An executable program is provided in the [supplementary material](#) for calculations. The GMM plot of the database is presented in the user interface as calculations are made. In this way, whether the calculations are within the ranges of the proposed database is visualized.

2.4. Support vector regression (SVR)

SVR provides the flexibility to define how much error is acceptable in the regression.²⁶ Deviations below a threshold, ε , are considered unimportant. In this way, a tube is defined of which the centerline is the prediction of the SVR model. Within the tube, deviations are not penalized in the objective function. The very idea of SVR is suitable for identifying datasets that present larger deviations compared to others. Advantages of SVR include that its generalization capability and prediction accuracy are excellent.²⁷ Therefore, SVR is very suitable for evaluating and correlating data of thermodynamic properties, for which extensive measurements are prohibitively expensive, and evenly distributed data are usually unavailable.

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

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

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

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

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

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

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

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

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

Equations (5) and (6) are transformed into the dual formula using the Lagrange multipliers,²⁸ α_i and α_i^* ,

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

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

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

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

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

In this work, the Gaussian kernel function²⁹ is used,

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

Predictions of a response at given x is calculated according to

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

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

- In the outer loop, the SVR hyperparameters, i.e., the box constraint, kernel scale, and threshold, ε , are optimized using the Bayesian optimization^{30–32} with the expected-improvement-plus algorithm³⁰ as the acquisition function to choose the next promising hyperparameter set, which is expected to have smaller errors for the validation set.
- In the inner loop, with fixed hyperparameters, the SVR model is optimized using the sequential minimal optimization algorithm.³³

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

The SVR model is used in both the evaluation and correlation of the database. In the evaluation, the entire database is used for training the SVR model in each step, as shown in Fig. 1(b).

In the correlation, the obtained reference database is split into training, validation, and test sets. For each solution, 20% of the data are set aside as test sets; the remaining 80% of the data are used as training/validation sets. 10-fold cross-validation is implemented for training the SVR models. The accuracy of the model on the training/validation and test sets are investigated. An executable program with user interface is provided in the [supplementary material](#) for calculations using the trained model.

2.5. Williams plot analysis

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

$$h_i = \mathbf{z}_i^T (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{z}_i, \quad (12)$$

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

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

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

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

3. Results and Discussion

The collected datasets are evaluated using the procedure explained in Sec. 2. [Table 2](#) provides the resulting reference database for the density of the 20 aqueous alkali halide solutions. 11 081 data points of 586 datasets from 309 references are included in the database. The references are provided in the table. We recommend that these references be cited when using the database. The full database is provided in the [supplementary material](#). As an example, the (water + KCl) system is discussed in detail here. The plots for the other aqueous alkali halide solutions are provided in the [supplementary material](#). [Figure 3](#) shows the GMM plot for the density data of the (water + KCl) system. The contour is to visualize data distribution. The GMM is analyzed on the $T - x_{\text{ion}}$ projection because most of the density data of the system are distributed at or near atmospheric pressure. The experimental data are plotted together with the contours.

Based on the database, an SVR model is developed according to the procedure introduced in Sec. 2.4. [Figure 4](#) shows the parity plot of the SVR correlation for the density of the (water + KCl) system. The test set is calculated with comparable accuracy to the training and validation sets. The SVR model is very accurate within the range of the database. Percentage average absolute deviation (AAD) and percentage maximum absolute deviation (MAD) for the 20 aqueous alkali halide solutions are provided in [Table 2](#). The deviations are slightly larger compared to the maximum deviations in the data evaluation step, in which the models are trained on all the data of the aqueous alkali halide solutions (maximum deviations between the selected datasets do not exceed 1%, and are smaller than 0.5% for most of the aqueous alkali halide solutions). We expect that training the SVR model based on the entire database would slightly improve correlation accuracy without hampering the extrapolation performance of the model. However, we would not be able to verify this without any data

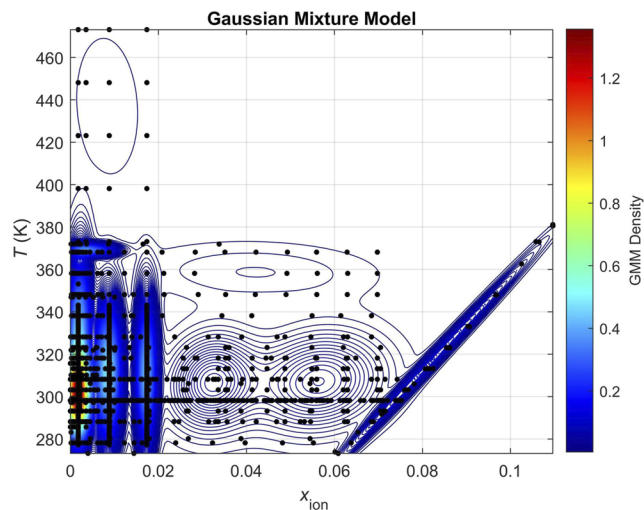


FIG. 3. Gaussian mixture model for the density data of the (water + KCl) system. The contour plot is the calculated data-distribution density. The dots are data points of the database.

for the test set. Therefore, 20% of the database is set aside as a test set.

[Figure 5](#) shows the Williams plot of the SVR correlation for the density data of the (water + KCl) system. There are some data points that exceed the threshold hat value. Most of these data points are at high pressure, while the majority in the database are at atmospheric pressure. However, deviations are not larger compared to the data points below the threshold. For the test set, the deviations are comparable to those of the training and validation sets. The good correlation and prediction show that the database is reliable on the edges of the data coverage, where there are much fewer data points,

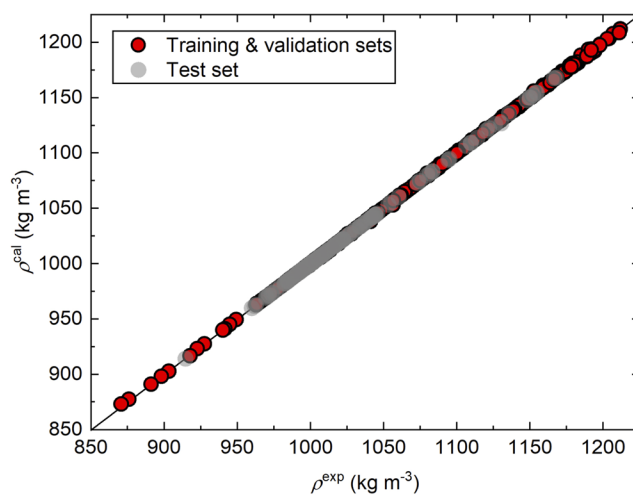


FIG. 4. Parity plot of the SVR correlation for the density of the (water + KCl) system.



FIG. 5. Williams plot of the SVR correlation for the density data of the (water + KCl) system. The hat values are calculated using Eq. (12) for the training and validation sets and for the test set.

and that the SVR model is not overfitted. The Williams plots for the SVR model of the other aqueous alkali halide solutions are provided in the [supplementary material](#). The behavior is similar to that of the (water + KCl) system.

An executable program is provided in the [supplementary material](#) for calculating density of the aqueous alkali halide solutions. Figure 6 shows an example of the user interface. Density results are provided along with data ranges of the solution, and illustrations of the calculations plotted on the Williams and GMM plots.

4. Conclusions

In this work, the experimental density data of 20 aqueous alkali halide solutions are extensively collected and critically evaluated using machine learning. A reference database consisting of 11 081 data points of 586 datasets from 309 references is constructed. Maximum deviations between the selected datasets do not exceed 1.1%, and are smaller than 0.5% for most of the aqueous alkali halide solutions. Data distribution is visualized using the Williams plot and Gaussian mixture model. Support vector regression models are developed based on the database and implemented in an executable program.

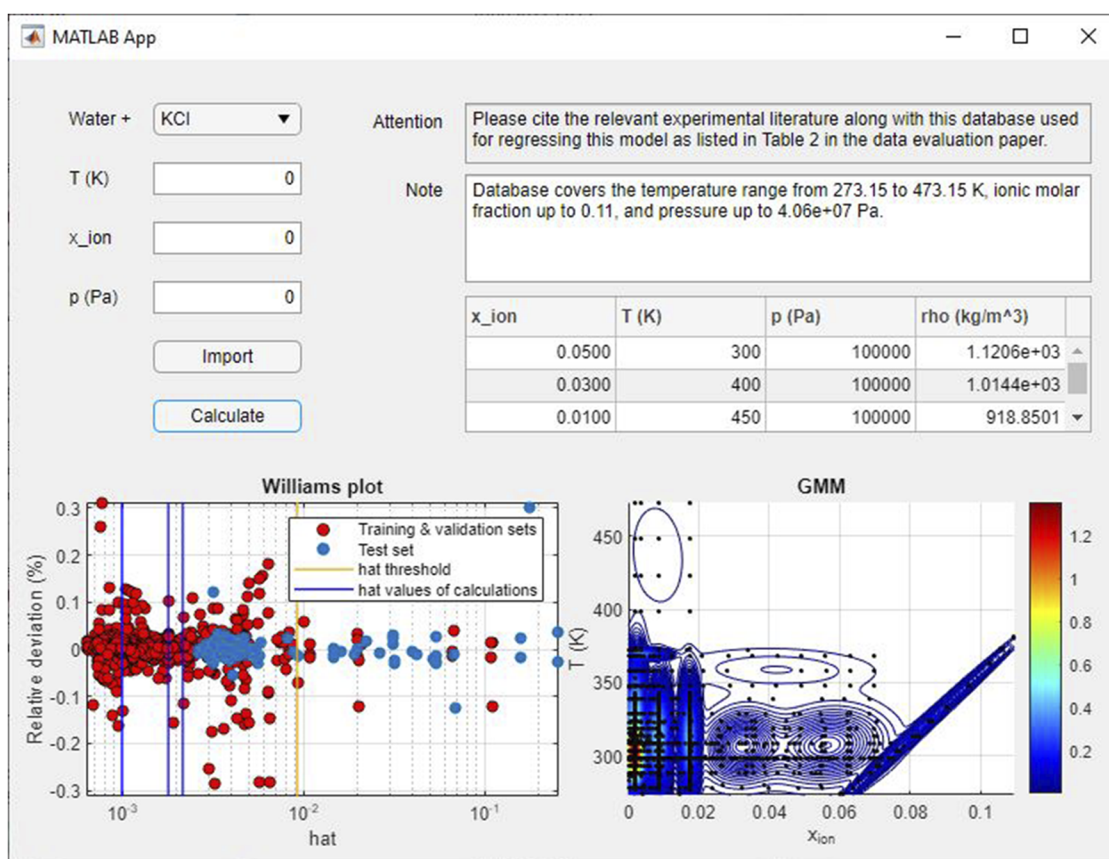


FIG. 6. Example of the user interface for density calculation. The salt is selected using the dropdown list on the top-left corner. Then, input can be made in the numeric edit fields, or imported from a file. A sample file is provided in the [supplementary material](#). Then, at the click of the "Calculate" button, results are shown in the table on the right side. Notes about the calculation are displayed above the table, summarizing ranges of the database for the mixture, or, in the case of a calculation beyond the database ranges, warnings about which input variable exceeds the range are displayed. The Williams and GMM plots are shown on the bottom.

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

5. Supplementary Material

The following are provided in the [supplementary material](#): An Excel file containing all the data, an executable program for density calculation, and the GMM and Williams plots for the aqueous alkali halide solutions.

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6. Author Declarations

6.1. Conflict of Interest

The authors have no conflicts to disclose.

7. Data Availability

The data that support the findings of this study are available within the article and its [supplementary material](#).

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