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Abstract: This work presents an analysis of various electrolyte SAFT model approaches through a rigorous benchmarking on extensively collected and critically evaluated databases. The primitive mean spherical approximation (MSA) and the Born equation are used respectively for the long-range ion-ion and ion-solvent interactions. For the short range interactions either dispersion, or association, or both (full) are investigated. Doing so, state-of-the-art parameter sets are obtained for the ePPC-SAFT model. Physical consistency is enforced for the parameters in the regression. Efforts are made to reduce the number of adjustable parameters with minimum loss of accuracy. This is done by analyzing the physical indication of the parameters, parameter sensitivity analysis, parameter trends, and trial-and-error. The model and parameter sets accurately represent the mean ionic activity coefficient (MIAC), vapor-liquid equilibria, and density, and accurately predict the osmotic coefficient extrapolated to temperature and salt composition ranges beyond the range of the MIAC data used in the regression. The ion-specific association strategies are found to be approximately as accurate as the salt-specific strategies, and are more accurate than the ion-specific dispersion and full strategies. Contributions of the model terms to the MIAC are analyzed. Temperature-dependence of the MIAC is discussed. The ion-specific association strategies successfully predicts the opposite relative magnitudes of the cation and anion individual ion activity coefficient of the aqueous NaCl and KCl solutions. The information is not included in model parameterization, while all the salt-specific strategies and ion-specific dispersion and full strategies fail. We recommend including the Wertheim association for the short-range ion-ion

and ion-solvent interactions, and parameterizing SAFT models in an ion-specific manner using physically consistent parameters.

Keywords: equation of state, aqueous electrolyte solutions, activity coefficient, vapor-liquid equilibria, density.

1 Introduction

Thermodynamics of electrolyte solutions is important in many industrial and chemical processes, e.g., carbon capture and sequestration [1], flue gas treatment [2], geochemical processes [3], desalination [4], and batteries [5,6]. When ions are present in mixtures, long-range ion-ion and ion-solvent interactions occur; thermodynamic properties of the electrolyte solutions are significantly different from those of molecular systems even at low salt concentration. Modeling these properties over ranges of temperature, pressure, and composition is important for the design and improvements of the relevant processes. Over the years, experimental data have been obtained for many electrolyte solutions; activity coefficient models and equations of state have been extended to mixtures involving electrolytes. In previous works [7–9], we have extensively collected and critically evaluated experimental thermodynamic property data of alkali halides in water and mixed-solvents. The databases cover various properties, including the mean-ionic activity coefficient (MIAC), vapor pressure, osmotic coefficient (OC), density, etc. Benchmarking the thermodynamic property models to these verified databases can help identify the contribution terms that are to be included in the models, the parameters that are to be regressed, and the properties that are to be included in the objective functions. The information will be useful when the models are applied on other electrolyte systems, for which experimental data are not as extensively available as for systems that have been covered by the reference databases.

Thermodynamics of electrolyte solutions has been reviewed in the literature, e.g., by Loehe and Donohue [10], Kontogeorgis et al. [11], Ahmed et al. [12], Held [13], etc. Activity coefficient models and equations of state (EoS) have been combined with electrolyte terms to account for the long-range ion-ion and ion-solvent interactions. There are a few works in which a non-primitive mean spherical approximation (MSA) model has been implemented [14–17], i.e., long-range ion-ion, ion-dipole, and dipole-dipole interactions are accounted for explicitly. The primitive MSA [18] or Debye-Hückel (DH) [19] theories are usually implemented in the EoS, in which the solvent is treated as a dielectric continuum. The ion-dipole and dipole-dipole interactions are accounted for using extra contribution terms in the EoS, e.g., the dispersion,

association, Born [20], and multipolar [21–23] terms. Maribo-Mogensen et al. [24] compared the MSA and DH theories, and concluded that they are similar within the EoS framework. In the following brief summary, a special focus would be on how the short-range interactions have been treated differently in the SAFT models, because benchmarking the short-range approaches is one of the goals of this work. The short-range interactions are modeled very differently in the literature:

- Some models use dispersion approach; some use the association approach; some use both; some use neither.
- In the dispersion approach, some models include like-ion dispersion; some do not include like-ion dispersion; some do not include ion-ion dispersion at all, but only include ion-water dispersion.
- In the association approach, some models include both cation-anion association and ion-water association; some only include ion-water association; some include cation-water association, but not anion-water association.

Galindo et al. [25] proposed the SAFT-VRE model, combining the SAFT-VR [26] with the MSA term. Ion-water dispersion was included, while ion-ion dispersion was not. Gil-Villegas et al. [27] compared the dispersion and association approaches for the short-range ion-water interaction. The Born term was added to the model as the model was applied on mixed-solvent electrolyte solutions [28]. Eriksen et al. [29] replaced the square-well dispersion term with the Mie potential. They included the dispersion interaction for the ion-ion and ion-water pairs, and the association interaction for the ion-water pairs. Liu et al. [30] extended a SAFT model to electrolyte solutions using a primitive MSA term. Later, cation-water association was included in the model, improving the results [31]; the MSA term was replaced using an expansion of the non-primitive MSA theory [32]. However, Das et al. [16] commented that the ion-solvent term in the low-density expansion reduced to the Born expression in the primitive MSA model. Cameretti et al. [33] combined the PC-SAFT model [34,35] with the DH term. Ion-solvent dispersion was included. Cation-anion dispersion was shown to improve results, while no like-ion dispersion was included [36]. Later on, the model was revised, adding composition dependent relative permittivity and the Born term [37]. Rozmus et al. [38] combined the PPC-SAFT model (a PC-SAFT revision with a multipolar term) with the MSA and Born terms. Association was included for the ion-ion and ion-solvent pairs. The model was revised with a temperature-dependent water diameter parameter, significantly improving the accuracy for liquid density, and was applied on mixed-solvent electrolyte solutions [12,39].

Roa Pinto et al. [40] investigated the temperature-dependence, short-range interactions, and relative permittivity models in the ePPC-SAFT framework. Association and dispersion approaches were compared for the short-range ion-ion and ion-solvent interactions. Like-ion dispersion was firstly included in the dispersion approach, and was removed in an attempt to reduce the number of adjustable parameters. The increasing mean ionic activity coefficient (MIAC) with temperature of the aqueous NaCl solution at low temperature was captured in the association approach. Maribo-Mogensen et al. [41] combined the CPA equation of state [42] with the DH theory. Walker et al. [43] compared the SAFT-VR Mie + DH and + MSA, and investigated the impact of the temperature-, density-, and composition-dependence of the relative permittivity model. Short-range ion-ion and ion-solvent interactions were modeled in the dispersion approach. Selam et al. [44] combined the SAFT-VR Mie model with the DH and Born terms. Both like- and unlike-ion dispersions were included. An attempt was made to capture the temperature-dependence of aqueous NaCl MIAC at low temperature using a temperature-dependent ion-water dispersion energy parameter. The model was applied on modeling gas solubility in aqueous electrolyte solutions [45].

The use of the readily available Wertheim association term for short-range ion-ion and ion-solvent interactions has been successful [28,31,40]. Wu and Prausnitz [46] stated that the Born term "gives only part of the change in Helmholtz energy due to charging neutral particles because the interaction between water and the charged particles also depends on the electrostatic states", and introduced "additional association interactions between ions and solvent (water) molecules to represent interactions between charged ions and water". However, when it comes to ion-ion interaction, the association decreases with temperature, contrary to the increasing trend of ion-pairing. As discussed in the last paragraph, the short-range interactions have been considered using very different assumptions, giving rise to the following questions:

- It has been assumed in some works that like-ion dispersion could be neglected. One could expect the like-ions to be far from each other, reducing this contribution. However, is the model "smart" enough to exclude dispersion between like-ions?
- Should dispersion, association, or both short-range interactions be used for ion-ion and ion-solvent interactions in the models? A full model would include both dispersion and association for the short-range ion-ion and ion-solvent interaction. After all, one could not assume associating ions to be free of dispersion interaction. However, the approach was rarely considered. With advanced algorithms, the increased number of parameters would

not pose difficulty in the regression. Would there be any improvements if the complete approach was considered?

- Can the experimental data be represented accurately without introducing physically inconsistent parameters?
- Is there any drawback in using the ion-specific parameters instead of salt-specific ones?

Following Ref [40], the ePPC-SAFT model is parameterized in this work in an ion-specific approach; physical consistency of parameters is enforced in the regression. State-of-the-art parameter sets are obtained to facilitate the benchmarking of the modeling approaches, based on extensively collected and critically evaluated databases. Efforts are made to reduce the number of parameters with minimum loss of accuracy. The final parameter set is determined based on analyzing the physical indication of the parameters, parameter sensitivity analysis, parameter trends, and trial-and-error. Ion-specific parameters are obtained within a series of alkali chloride aqueous solutions. Properties that are useful in practical applications are included in the objective function, i.e., MIAC, vapor-liquid equilibria (VLE), and density. In future works, the model will be extended to mixed-solvent electrolyte solutions. The osmotic coefficient is not included in the regression, but is used as a validation of the model and parameter set. Efforts are made to improve density correlation, using our previously evaluated reference database for aqueous alkali halide solutions [9]. The association, dispersion, and full approaches are compared. In the dispersion and full approaches, the effect of the like-ion dispersion is investigated. The obtained ion-specific parameter sets are tested on the qualitative behavior of cation and anion individual ion activity coefficients (IIAC) of aqueous NaCl and KCl solutions. It is observed that the respective magnitudes of the cation and anion IIAC is opposite for the 2 aqueous solutions. This phenomenon has never been successfully predicted in the literature. The manuscript is organized as follows. In Section 2, the model, database, and parameterization strategies for the short-range ion-ion and ion-solvent interactions are introduced. In Section 3, comparisons are presented for the dispersion, association, and full strategies, and for the salt- and ion-specific parameterizations. In Section 4, contributions of the terms are investigated; of the MIAC temperature dependence represented using the model and parameter sets is shown; the model is validated using the osmotic coefficient and individual ion activity coefficient, which have not been used in the parameterization, In Section 5, concluding remarks are presented.

2 Method

In this section, the model, database, salt- and ion-specific parameterization strategies, and the different parameterization strategies for the short-range ion-ion and ion-solvent interactions are introduced.

2.1 ePPC-SAFT

In the ePPC-SAFT model [12,38–40], the residual Helmholtz energy is given as,

$$A^{\mathrm{res}} = A^{\mathrm{hc}} + A^{\mathrm{disp}} + A^{\mathrm{assoc}} + A^{\mathrm{polar}} + A^{\mathrm{MSA}} + A^{\mathrm{Born}} \tag{1}$$

where the superscript hc denotes hard-chain, disp denotes dispersion, assoc denotes association, polar denotes multipolar as presented by Ref [21–23]. For details about the equations for each term and the adjustable parameters (unary and binary), please refer to Ref [12,40]. Here the electrolyte terms of the model are briefly introduced.

The primitive MSA is used for describing the long-range interaction between cation and anion.

$$A^{\mathrm{MSA}} = -\frac{N_{\mathrm{A}} {q_{\mathrm{e}}}^2}{4\pi\varepsilon_0\varepsilon_{\mathrm{r}}} \sum_{\mathrm{ions}} \frac{n_i {Z_i}^2 \Gamma}{1 + \Gamma\sigma_i^{\mathrm{MSA}}} + \frac{\Gamma^3 RT}{3\pi\rho N_{\mathrm{A}}} \tag{2}$$

$$\Gamma^2 = \frac{{q_{\mathrm{e}}}^2 {N_{\mathrm{A}}}^2}{4\varepsilon_0\varepsilon_{\mathrm{r}}RT} \sum_{\mathrm{ions}} n_i\rho \left[\frac{Z_i}{1 + \Gamma\sigma_i^{\mathrm{MSA}}}\right]^2 \tag{3}$$

where N_{A} is the Avogadro constant, q_{e} is the elementary charge, ε_0 is the dielectric constant in the vacuum, ε_{r} is the relative permittivity, n_i is the number of moles of ion i, Z_i is the ionic valence, σ_i^{MSA} is the MSA diameter, R is the universal gas constant, T is temperature, and ρ is density.

The Born term is given in the usual form:

$$A^{\mathrm{Born}} = \frac{N_{\mathrm{A}} {q_{\mathrm{e}}}^2}{4\pi\varepsilon_0 RT}\left(1 - \frac{1}{\varepsilon_{\mathrm{r}}}\right) \sum_{\mathrm{ions}} \frac{n_i {Z_i}^2}{\sigma_i^{\mathrm{Born}}} \tag{4}$$

where σ_i^{Born} is the Born diameter. The Born diameter is calculated using the Born term and the experimental Gibbs energy of solvation obtained by Ref [47]. According to Ref [40], obtaining

the Born diameter in this way ensures accurate representation of the Gibbs energy of solvation of the ePPC-SAFT model.

The relative permittivity models shown in Ref [28] and [48] are used in this work, denoted as RPM-1 and RPM-2, respectively. In RPM-1, the salt-composition dependence is accounted for only via the density:

$$\varepsilon_r = 1 + \frac{n_{\text{solv}}}{V} d_v \left(\frac{d_T}{T} - 1 \right) \tag{5}$$

where n_{solv} is the number of moles of the solvent of volume V, $d_v = 0.3777\ \text{dm}^3/\text{mol}$ and $d_T = 1403\ \text{K}$ for water [28].

In RPM-2, an additional correction factor is applied for the salt composition dependence:

$$\varepsilon_r = 1 + (\varepsilon_{r0} - 1) \frac{1 - \xi}{1 + \frac{\xi}{2}} \tag{6a}$$

$$\xi = \frac{N_A \pi}{6} \sum_{\text{ions}} \frac{n_i {\sigma_i^{\text{HS}}}^3}{V} \tag{6b}$$

where ε_{r0} is calculated using RPM-1, and σ_i^{HS} is the ionic hard sphere diamter.

One should note that neither of these models represents accurately the experimental salt composition dependence of the relative permittivity, as shown in Figure 1. The needed solutions density and ionic diameters are from a preliminary parameter set. In Roa Pinto et al.'s work [40], Simonin's empirical model [49] was also investigated, with the adjustable parameters regressed along with the ionic parameters of the ePPC-SAFT model. However, the resulting relative permittivity approached the RPM-1 rather than the experimental data, indicating that the RPM that is needed in the EoS should present a much less drastic decrease compared to the experimental data. In addition, Maribo-Mogensen et al. [50] suggested that the kinetic depolarization part of the relative permittivity, which was more than half of the observed decrease (Figure 1 in Ref [50]), was a dynamic property, and should not be included in the thermodynamic modeling of electrolytes. Therefore, the observed significant overestimations via RPM-1 and -2 compared to the experimental RP data maybe partially justified.

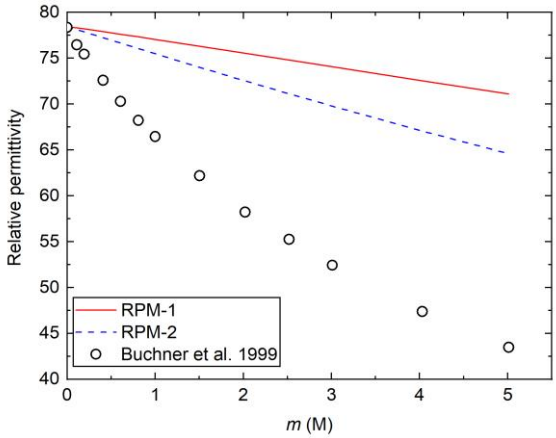

Figure 1. Comparison of the RPMs with the experimental relative permittivity data of aqueous NaCl solution [51].

For water, the parameter set from Ref [39] is used. Unlike other implementations of the PC-SAFT models, the sphere softness was made adjustable for water rather than fixed at 0.12. Parameters were regressed over liquid densities and vapor pressure pure water from 273.15 to 550 K and on the LLE of (water + n-alkane) mixtures. The abnormal behavior of water density was captured using a temperature dependent segment diameter:

$$\sigma_{\mathrm{w},T} = \sigma_{\mathrm{w}} + n_{T_1} e^{n_{T_2} T} + \frac{n_{T_3}}{T^2} \tag{7}$$

Ionic parameters are regressed to thermodynamic properties of aqueous solutions of the salts, as will be explained in detail in the following sections.

2.2 Objective function and reference database

In this work, aqueous solutions of 4 alkali chloride salts (NaCl, KCl, RbCl, and CsCl) are investigated. Mean-ionic activity coefficient (MIAC, $\gamma^{\pm}$), vapor-liquid equilibria (VLE), and density are included in the objective function:

$$\mathrm{OF} = \frac{1}{2}\frac{\sum_{i=1}^{n_{\mathrm{dp}}^{\gamma^{\pm}}}\left(\frac{\gamma^{\pm}{}_{\mathrm{cal}} - \gamma^{\pm}{}_{\mathrm{exp}}}{\gamma^{\pm}{}_{\mathrm{exp}}}\right)^2}{n_{\mathrm{dp}}^{\gamma^{\pm}}} + \frac{1}{2}\frac{\sum_{i=1}^{n_{\mathrm{dp}}^{p}}\left(\frac{p_{\mathrm{cal}} - p_{\mathrm{exp}}}{p_{\mathrm{exp}}}\right)^2}{n_{\mathrm{dp}}^{p}} + \frac{1}{2}\frac{\sum_{i=1}^{n_{\mathrm{dp}}^{\rho}}\left(\frac{\rho_{\mathrm{cal}} - \rho_{\mathrm{exp}}}{\rho_{\mathrm{exp}}}\right)^2}{n_{\mathrm{dp}}^{\rho}} \tag{8}$$

where n_{dp} is the number of data points of the property, p is the VLE pressure. The MIAC reference state is at infinite dilution in the aqueous solution in the molality unit. The involved

reference states and conventions, and equations for deriving them from the EoS have been explained in [7–9,40].

The data used in the regression are from the evaluated databases in our previous works [8,9]. In the data evaluation, datasets that contain outliers have been removed. Table 2 shows the information for each property of each aqueous electrolyte solution. The data used in the regression are: for MIAC from Ref [52–78]; for VLE from Ref [79–91]; for density from Ref [81,92–298]. The osmotic coefficient is not used in the objective function, but is used for validating the obtained model and parameter sets. The osmotic coefficient data have been evaluated in Ref [7].

Table 1. Number of datasets, number of data points, and ranges for each property of each aqueous electrolyte solution used in the parameter regression in this work.

Water +	Property	No. datasets	No. data points	T (K)	x_{ion}
NaCl	MIAC	20	344	273.15~333.15	~0.089
	VLE	3	166	294.34~368.07	~0.091
	Density	129	2578	253.00~473.15	~0.098
KCl	MIAC	4	43	273.15~298.15	~0.056
	VLE	8	192	298.15~374.15	~0.095
	Density	104	1615	273.15~473.15	~0.11
RbCl	MIAC	1	21	298.15	~0.076
	VLE	3	65	303.15~368.15	~0.10
	Density	14	168	288.15~328.15	~0.12
CsCl	MIAC	4	51	298.15	~0.049
	VLE	2	75	303.15~368.15	~0.12
	Density	30	351	273.85~473.15	~0.19

2.3 Salt-specific parameterization

Both salt- and ion-specific parameterizations are investigated in this work. Here, the adjustable parameters of the ions for the salt-specific strategies are explained. The number of parameters are reduced to facilitate ion-specific parameterization in the next step, as will be explained in Section 2.4.

Efforts are made to improve density accuracy by including the suitable volumetric parameters in the regression in this work. In a comparison of an electrolyte SAFT-VR model with Monte Carlo simulations, Zhao et al. [14] showed that, when the primitive MSA model was used, using the Pauling diameters as the ionic diameters resulted in systematic deviations

of density results. Therefore, the ionic hard sphere (HS) diameters are adjusted in this work. To ensure the "correct order" of the ionic HS diameters, it is assumed that they are proportional to the Pauling diameters [299]; the ratio (r^{HS}) of the HS diameter over the Pauling diameter, Eq. (9), is regressed instead of the diameters themselves. The same value is taken for the cation and anion in the salt-specific parameterization. To conveniently enforce the constraint that the MSA diameter has to be larger than the HS diameter, the ratio (r^{MSA}) of the MSA diameter over the HS diameter, Eq. (10), is regressed rather than the diameters themselves. Roa Pinto et al. [40] showed that, the ePPC-SAFT model accurately reproduced the Gibbs energy of solvation when the Born diameters were calculated based on the Born term alone. In this work, the same approach is taken for the Born diameters. Ionic Pauling diameters and Born diameters are provided in the Supplementary Material.

$$r^{\mathrm{HS}} = \frac{\sigma^{\mathrm{HS}}}{\sigma^{\mathrm{Pauling}}} \tag{9}$$

$$r^{\mathrm{MSA}} = \frac{\sigma^{\mathrm{MSA}}}{\sigma^{\mathrm{HS}}} \tag{10}$$

As discussed in Section 1, in addition to the MSA or DH term for the long-range ion-ion interaction and the Born term for the long-range ion-solvent interaction, different approaches have been investigated for the short-range ion-ion and ion-solvent interactions. In this work, 10 parameterization strategies are compared for the aqueous NaCl solution, as shown in Table 2. In the following text, the abbreviations (Disp-1, Assoc-1, Full-1, etc.) are used for denoting the parameterization strategies. r^{HS} and r^{MSA} are regressed for all strategies. For the dispersion strategies, the dispersion term is used for describing the short-range ion-ion and ion-solvent interactions. Hence, the dispersion energy of the cation and anion (ε_{c} and ε_{a}), and the binary interaction parameter between the cation and anion ($k_{\mathrm{c-a}}$) are also regressed. The dispersion energy between the cation and water ($\varepsilon_{\mathrm{c-w}}$), between the anion and water ($\varepsilon_{\mathrm{a-w}}$), and between the cation and anion ($\varepsilon_{\mathrm{c-a}}$) are obtained using Eq. (11). No binary interaction parameter is used for the ion-water dispersion interaction. When like-ion dispersion is not included, $\varepsilon_{\mathrm{c-c}}$ and $\varepsilon_{\mathrm{a-a}}$ are artificially set at 0. Naturally, when like-ion dispersion is included, $\varepsilon_{\mathrm{c-c}} = \varepsilon_{\mathrm{c}}$, and $\varepsilon_{\mathrm{a-a}} = \varepsilon_{\mathrm{a}}$.

$$\varepsilon_{\mathrm{i-w}} = \sqrt{\varepsilon_{\mathrm{i}}\varepsilon_{\mathrm{w}}} \tag{11a}$$

$$\varepsilon_{\mathrm{c-a}} = \sqrt{\varepsilon_{\mathrm{c}}\varepsilon_{\mathrm{a}}}(1 - k_{\mathrm{c-a}}) \tag{11b}$$

For the association strategies, the Wertheim association term is used for describing the short-range ion-ion and ion-solvent interactions. The number of association sites is set to 7 for the cation, and 6 for the anion, same as in previous works [12,40]. Hence, the association energy parameters of the cation and anion ($\varepsilon_{\mathrm{c}}^{\mathrm{AB}}$ and $\varepsilon_{\mathrm{a}}^{\mathrm{AB}}$), and the binary interaction parameter between the anion and cation ($w_{\mathrm{c-a}}$) are regressed. The association interaction is included between water and water, ion and water, and cation and anion. The cross-association energies ($\varepsilon_{\mathrm{c-w}}^{\mathrm{AB}}$, $\varepsilon_{\mathrm{a-w}}^{\mathrm{AB}}$, and $\varepsilon_{\mathrm{c-a}}^{\mathrm{AB}}$) are obtained using Eq. (12). The association volumes of the cation ($\beta_{\mathrm{c}}^{\mathrm{AB}}$) and anion ($\beta_{\mathrm{a}}^{\mathrm{AB}}$) are also regressed. The cross-association volume is obtained using Eq. (13). No binary interaction parameter is included for the unlike-ion association volume.

$$\varepsilon_{\mathrm{i-w}}^{\mathrm{AB}} = \left(\varepsilon_{\mathrm{i}}^{\mathrm{AB}} + \varepsilon_{\mathrm{w}}^{\mathrm{AB}}\right)/_{2} \tag{12a}$$

$$\varepsilon_{\mathrm{c-a}}^{\mathrm{AB}} = (\varepsilon_{\mathrm{c}}^{\mathrm{AB}} + \varepsilon_{\mathrm{a}}^{\mathrm{AB}})(1 - w_{\mathrm{c-a}})/_{2} \tag{12b}$$

$$\beta_{ij}^{\mathrm{AB}} = \sqrt{\beta_i^{\mathrm{AB}}\beta_j^{\mathrm{AB}}} \tag{13}$$

For the full strategies, both the dispersion and Wertheim association terms are used for describing the short-range ion-ion and ion-solvent interactions. Hence, the parameter set also includes ε_{c}, ε_{a}, $\varepsilon_{\mathrm{c}}^{\mathrm{AB}}$, $\varepsilon_{\mathrm{a}}^{\mathrm{AB}}$, $w_{\mathrm{c-a}}$, $\beta_{\mathrm{c}}^{\mathrm{AB}}$, and $\beta_{\mathrm{a}}^{\mathrm{AB}}$. In order to keep the number of adjustable parameters reasonable, no binary interaction parameter is included for the unlike-ion dispersion energy and association volume. We notice that there is a different sensitivity of the cation and anion energy parameters (dispersion or association). Furthermore, the solvation effect of the cation and anion are very different as reported in nuclear magnetic resonance measurements [300] and molecular simulations [301]. Liu et al. [30] included cation-solvent association, but excluded anion-solvent association in their electrolyte SAFT model. However, from an engineering perspective, we find this sensitivity to be case-specific in the parameter sensitivity analysis. Furthermore, removing one of the ionic interaction parameters would place a strong impact on the individual ion activity coefficient results. Therefore, both the cation-water and anion-water interactions are included. Regression boundaries of the parameters are provided in the Supplementary Material.

Table 2. Salt-specific parameterization strategies.

	Solvent-ion	Ion-ion	RPM-	Like-ion dispersion	Parameters
Disp-1	Dispersion, Born	Dispersion, MSA	1	No	5: ε_{c}, ε_{a}, $k_{\mathrm{c-a}}$, r^{HS}, r^{MSA}
Disp-2			2		
Disp-3			1	Yes	
Disp-4			2		
Assoc-1	Association, Born	Association, MSA	1	-	7: $\varepsilon_{\mathrm{c}}^{\mathrm{AB}}$, $\varepsilon_{\mathrm{a}}^{\mathrm{AB}}$, $\beta_{\mathrm{c}}^{\mathrm{AB}}$, $\beta_{\mathrm{a}}^{\mathrm{AB}}$, $w_{\mathrm{c-a}}$, r^{HS}, r^{MSA}
Assoc-2			2		
Full-1	Dispersion, association, Born	Dispersion, association, MSA	1	No	9: ε_{c}, ε_{a}, $\varepsilon_{\mathrm{c}}^{\mathrm{AB}}$, $\varepsilon_{\mathrm{a}}^{\mathrm{AB}}$, $\beta_{\mathrm{c}}^{\mathrm{AB}}$, $\beta_{\mathrm{a}}^{\mathrm{AB}}$, $w_{\mathrm{c-a}}$, r^{HS}, r^{MSA}
Full-2			2		
Full-3			1	Yes	
Full-4			2		

One might argue that comparisons are only fair with the same number of adjustable parameters. However, the larger number of adjustable parameters and the resulting advantage of being more flexible are intrinsic in the association and full strategies. Therefore, no effort has been made to compare the strategies based on the same number of adjustable parameters. Furthermore, as will be shown in Section 3, the Full strategies do not provide better results despite using a larger number of adjustable parameters. In addition, as will be shown in Section 2.4, the ion-specific strategies will be compared using the same number of adjustable parameters.

Parameters are regressed using an evolutionary algorithm [302], which is helpful for avoiding local minima. In the salt-specific parameterization, different Cl^- parameters are taken for each salt. The regressed salt-specific parameters for the 4 salts are provided in the Supplementary Material. The resulting deviations will be discussed in Section 3.

For the aqueous NaCl solution, all 10 strategies are used. For Disp-3 and -4, the dispersion energy parameters are too large (ε/k is approximately 1000 K for Na^+ compared to 201.747 K for water), the binary interaction parameter, $k_{\mathrm{c-a}}$, is close to 1 (the upper boundary), while the accuracy is lower compared to the other strategies. Therefore, these two dispersion strategies are not further pursued for the other aqueous electrolyte solutions, while the remaining 8 strategies are investigated for the other 3 salts. At this point, we have partly addressed the question posted earlier "Is the model "smart" enough to exclude dispersion between like-ions?" For the dispersion strategies, yes: $k_{\mathrm{c-a}} = 1$ indicates zero dispersion between unlike-ions, which is not reasonable with a non-zero dispersion between like-ions. However, the full

strategies with (Full-3 and -4) and without (Full-1 and -2) like-ion dispersion do not present such distinction, with Full-3 and -4 presenting slightly better trend in parameters and higher accuracy than Full-1 and -2.

The parameters r^{HS} and r^{MSA} are the only ones that present trends with the cations in the salt-specific regressions. Figure 2 shows the regressed r^{HS} and r^{MSA} in the salt-specific strategies, Assoc-1, Assoc-2, Disp-1, Disp-2, Full-3, Full-4. r^{HS} is approximately the same for the 4 alkali chlorides in each of the parameterization strategies. In most of the cases, r^{HS} is smaller than 1, i.e., the HS diameter is smaller than the Pauling diameter, and is very close to 1 in a few cases of the full strategies. r^{HS} is approximately 0.8 in the dispersion strategies, and is in general between 0.93 and 1 in the association and full strategies. In Ref [40], r^{MSA} was set at 1.5 for the aqueous NaCl solution in order to reduce the number of adjustable parameters. The value agrees with the regressed r^{MSA} in this work. For the heavier cations, however, the regressed r^{MSA} is smaller. For CsCl, r^{MSA} reaches 1 (regression lower boundary) in some of the cases; deviations are larger compared to the other salts (as will be shown in Sections 3 and 4), and can be reduced given a r^{MSA} that is smaller than 1. For RbCl, r^{MSA} is also 1 or very close to 1 in the dispersion strategies. The parameter behavior might have resulted from certain assumptions in the SAFT, MSA, and Born terms. In addition, the contributions except for that of the MSA term are all close to linear, and compensate for each other, as will be shown in Section 4.1. As will be shown in Section 3, deviations in VLE are also larger compared to the association strategies, presenting another reason for preferring the association strategies over the dispersion strategies. However, the boundary is set at 1 regardless of this potential slight accuracy improvement, to avoid the inconsistency of smaller MSA diameters than the HS diameters. The value of r^{HS} is approximately the same for the 4 salts in each of the strategies, while r^{MSA} is smaller for the heavier salts. Therefore, in the ion-specific parameterization, the same r^{HS} is used for all 5 ions, while different r^{MSA} are used for each ion, as will be discussed in the next section.

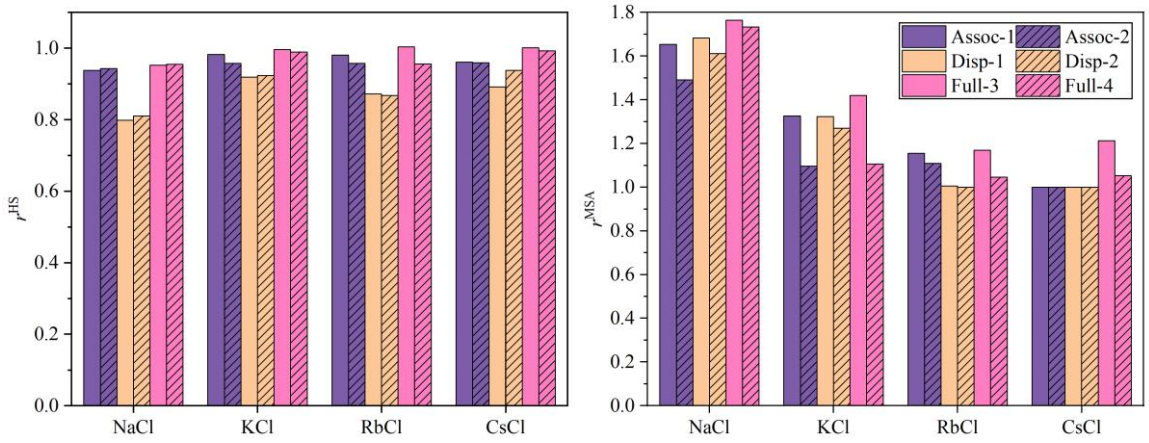

Figure 2. Regressed r^{HS} (left) and r^{MSA} (right) in the salt-specific strategies Assoc-1, Assoc-2, Disp-1, Disp-2, Full-3, and Full-4.

Furthermore, the response surface is analyzed so that the number of adjustable parameters could be reduced with minimum loss in accuracy. Figure 3 shows the response surface of the objective function, Eq. (8), over the parameters in the salt-specific strategy, Assoc-1, for the aqueous NaCl solution. Contours are plotted on the same levels over r^{HS} and each of the other parameters. Obviously, there is parameter degeneracy. r^{HS}, $w_{\mathrm{c-a}}$ and r^{MSA} are the most pronounced parameters, while the association energy and volume parameters are less pronounced. The "valleys" are almost parallel to the association volume axis, indicating that the objective function is not sensitive to these parameters. The behavior is similar for the other aqueous electrolyte solutions. Therefore, $\beta_{\mathrm{c}}^{\mathrm{AB}}$ and $\beta_{\mathrm{a}}^{\mathrm{AB}}$ are fixed to that of water in the ion-specific parameterization. Although the "valley" is also parallel to the $\varepsilon_{\mathrm{c}}^{\mathrm{AB}}/k$ axis, the situation is case-specific. Therefore, the association energy parameters are kept adjustable in the ion-specific parameterization.

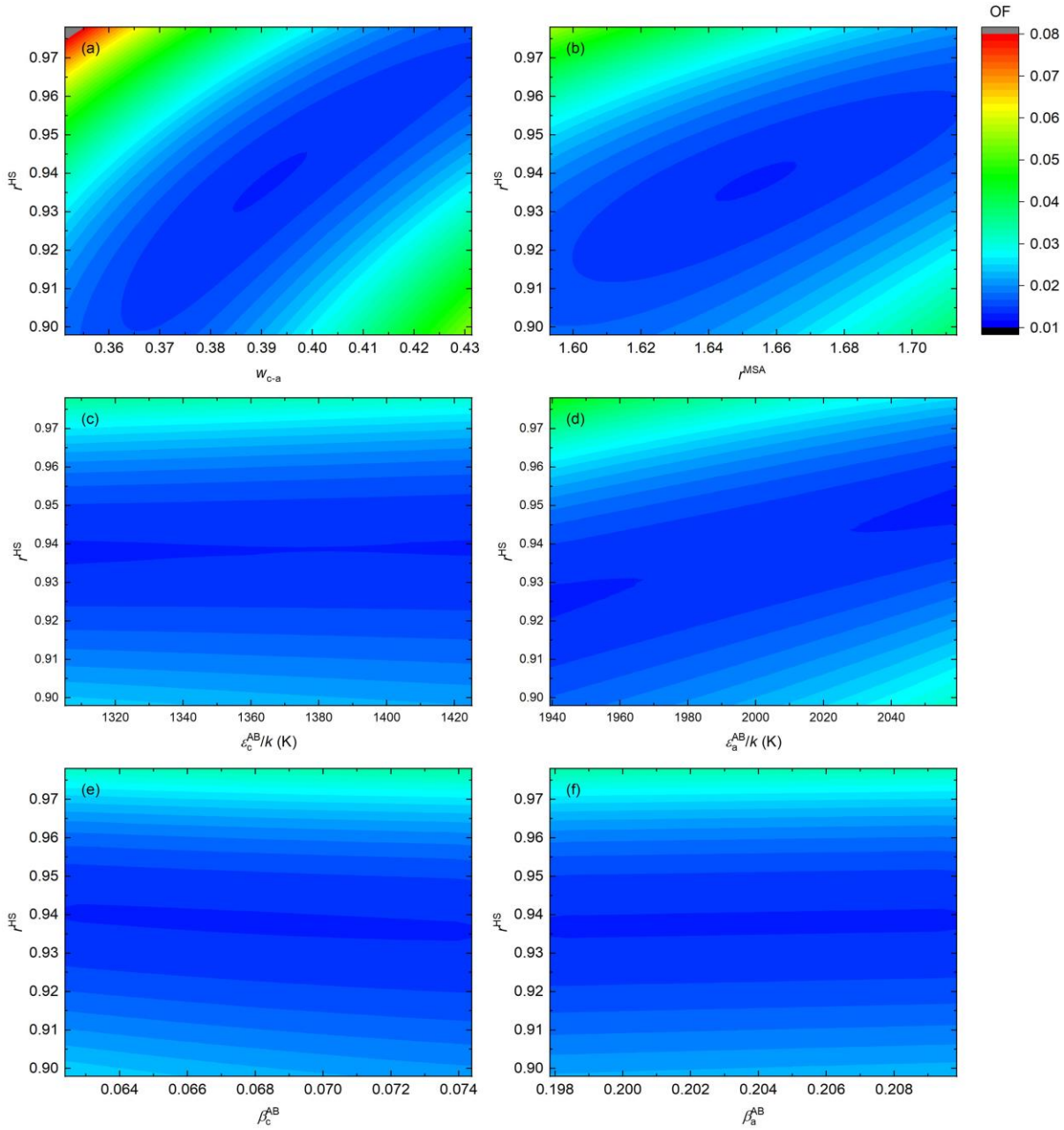

Figure 3. Response surface of the objective function, Eq. (8), as a function of the parameters in the salt-specific strategy , Assoc-1, for the aqueous NaCl solution: (a) r^{HS} - $w_{\mathrm{c-a}}$, (b) r^{HS} - r^{MSA}, (c) r^{HS} - $\varepsilon_{\mathrm{c}}^{\mathrm{AB}}/k$, (d) r^{HS} - $\varepsilon_{\mathrm{a}}^{\mathrm{AB}}/k$, (e) r^{HS} - $\beta_{\mathrm{c}}^{\mathrm{AB}}$, (f) r^{HS} - $\beta_{\mathrm{a}}^{\mathrm{AB}}$. In all the sub-graphs, all the other parameters are fixed at their optimal values.

2.4 Ion-specific parameterization

Ion-specific parameterization is desirable because it facilitates simple extension to mixed-salt systems, as no mixing rule is needed for the parameters of the same ion from different salts. Furthermore, it could potentially bring in information about the contributions of the cation and anion to the mean properties, even though individual ion information is not sufficiently included in the parameterization. However, obtaining these parameters requires regressing the parameters of a series of electrolyte solutions simultaneously [11]. Therefore, in this work,

efforts have been made to reduce the number of adjustable parameters with minimum loss in accuracy compared to the salt-specific parameterization, based on the findings in the salt-specific parameterization.

Table 3 shows the ion-specific parameterization strategies, abbreviated as Assoc-I-X, Disp-I-X, and Full-I-X, where the symbol "X" indicates the number of adjustable parameters. At first, the 15-parameter scenarios are investigated. Thus, the resulting ion-specific association strategy is Assoc-I-15, including the parameters, r^{HS}, 5 r^{MSA} for the 5 ions, 4 $w_{\mathrm{c-a}}$ for the 4 salts, and 5 $\varepsilon_{\mathrm{i}}^{\mathrm{AB}}$ for the 5 ions. Similarly, for Disp-I-15, the 4 $k_{\mathrm{c-a}}$ and 5 ε_{i} parameters are optimized instead of their association counterparts; for Full-I-15, the parameter set is the same as Assoc-I-15, the ε_{i} parameters are set at the water value, while $k_{\mathrm{c-a}}$ is set at 0. Like-ion dispersion is excluded in the dispersion strategies, but is included in the full strategies, according to the discussions in Section 2.3. Regression boundaries of the parameters are provided in the Supplementary Material. Rather than obtaining the parameters incrementally, i.e., starting from one of the salts and extending to the others, the 15 parameters are optimized simultaneously to the thermodynamic property data of the 4 aqueous alkali halide solutions. This facilitates a genuine ion-specific parameterization, as the contributions of the cation and anion are introduced into the regression by the difference of the mean thermodynamic property data of the 4 aqueous electrolyte solutions. In addition, compared to using salt-specific parameters of a reference system and extending to other salts that share a common ion (for instance, using the Cl^- parameters from NaCl and extending to other Cl^- salts), this approach avoids preferring over the accuracy of the reference system in the incremental approach while compromising that of the other systems.

Table 3. Parameter sets for the ion-specific strategies, including 4 cations (Na^+, K^+, Rb^+, and Rb^+) and 1 anion (Cl^-).

	Parameter set
Assoc-I-15	15: r^{HS}, 5 r^{MSA} for the 5 ions, 4 $w_{\mathrm{c-a}}$ for the 4 salts, and 5 $\varepsilon_{\mathrm{i}}^{\mathrm{AB}}$ for the 5 ions
Assoc-I-12	12: r^{HS}, 5 r^{MSA} for the 5 ions, $w_{\mathrm{c-a}}$, and 5 $\varepsilon_{\mathrm{i}}^{\mathrm{AB}}$ for the 5 ions
Disp-I-15	15: r^{HS}, 5 r^{MSA} for the 5 ions, 4 $k_{\mathrm{c-a}}$ for the 4 salts, and 5 ε_{i} for the 5 ions
Disp-I-12	12: r^{HS}, 5 r^{MSA} for the 5 ions, $k_{\mathrm{c-a}}$, and 5 ε_{i} for the 5 ions
Full-I-15	15: r^{HS}, 5 r^{MSA} for the 5 ions, 4 $w_{\mathrm{c-a}}$ for the 4 salts, and 5 $\varepsilon_{\mathrm{i}}^{\mathrm{AB}}$ for the 5 ions
Full-I-12	12: r^{HS}, 5 r^{MSA} for the 5 ions, $w_{\mathrm{c-a}}$, and 5 $\varepsilon_{\mathrm{i}}^{\mathrm{AB}}$ for the 5 ions
Full-I-20	20: r^{HS}, 5 r^{MSA} for the 5 ions, 4 $w_{\mathrm{c-a}}$ for the 4 salts, 5 $\varepsilon_{\mathrm{i}}^{\mathrm{AB}}$ for the 5 ions, and 5 ε_{i} for the 5 ions

In a next step, efforts are made to reduce the number of adjustable parameters. First, the same ε_c^{AB} is regressed using a single parameter for all cations, reducing the number of adjustable parameters from 15 to 12. However, even though the accuracy is as good as the 15-parameter strategies, the individual ion activity coefficient (IIAC) is predicted to be smaller for cation than for anion for both the aqueous NaCl and KCl solutions, i.e., the model and parameter set fail in predicting the opposite relative magnitudes of cation and anion IIAC for aqueous NaCl and KCl solutions. To obtain the qualitatively correct behavior, different association energy parameters have to be used for Na^+ and K^+. Therefore, it is attempted to use the same w_{c-a} for the 4 aqueous solutions, reducing the number of adjustable parameters from 15 to 12. The 12-parameter ion-specific association strategy is denoted as Assoc-I-12. Similarly, the numbers of parameters for the dispersion and full ion-specific strategies are reduced from 15 to 12; the 12-parameter strategies are denoted as Disp-I-12 and Full-I-12.

Unlike the salt-specific cases, results of Full-I-15 and Full-I-12 are much worse than Assoc-I-15 and Assoc-I-12. It is suspected that the increased deviations result from the fixed dispersion energy parameter. Therefore, the dispersion energy parameters of the 5 ions are included in the ion-specific full strategy, i.e., Full-I-20.

In the salt-specific cases, using RPM-1 or -2 results in only marginally different results. Therefore, RPM-1 is used in all the ion-specific cases; the impact of the relative permittivity model is not further pursued in this work.

The regressed parameters of the ion-specific strategies are provided in the Supplementary Material. Like in the salt-specific cases, r^{HS} is smaller for the dispersion strategies than for the association and full strategies. Figure 4 shows the regressed r^{MSA} in the ion-specific strategies, Assoc-I-15, Assoc-I-12, Disp-I-15, Disp-I-12, Full-I-15, Full-I-12, and Full-I-20. For all the strategies except for Full-I-12, r^{MSA} decreases with ionic size within the cations. In all ion-specific strategies, r^{MSA} is 1 for Cs^+. Accuracy could be improved if the constraint that the MSA diameter must be larger than the HS diameter is relaxed. However, it is decided not to do so. For Disp-I-15, Disp-I-12, Full-I-15, and Full-I-12, r^{MSA} is also 1 for Cl^-. These strategies also result in larger deviations compared to the others, as will be discussed in Section 3.2.

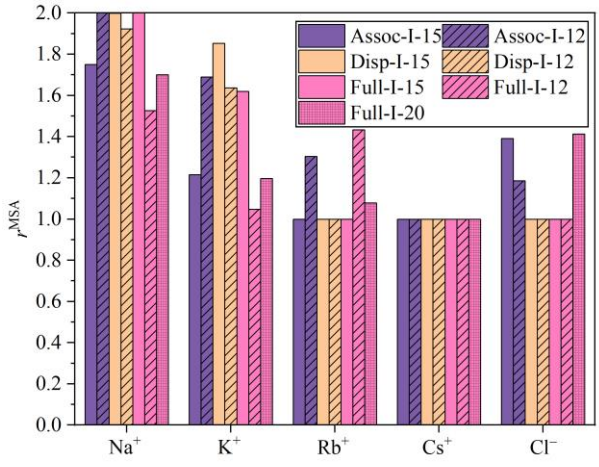

Figure 4. Regressed r^{MSA} in the ion-specific strategies, Assoc-I-15, Assoc-I-12, Disp-I-15, Disp-I-12, Full-I-15, Full-I-12, and Full-I-20.

3 Results

In this section, we compare the salt-specific association, dispersion, and full strategies as well as the ion- and salt-specific strategies approaches.

3.1 Comparison of the dispersion, association, full strategies for the short-range ion-ion and ion-solvent interactions

The percentage average absolute deviations (AADs) and percentage maximum absolute deviations (MADs) of the salt-specific strategies for the 4 aqueous electrolyte solutions are shown in Table 4. For all 4 salts, the association and full strategies are more accurate than the dispersion strategies. Therefore, it appears necessary to include the association term for the short-range ion-ion and ion-solvent interactions. For the aqueous NaCl solution, Disp-3 and -4, in which like-ion dispersion is included, present slightly larger MADs compared to Disp-1 and Disp-2, in which like-ion dispersion is excluded. Unlike the dispersion strategies, whether the like-ion dispersion is accounted for does not significantly affect the result for the full strategies. Considering the unreasonable parameters of Disp-3 and -4, as discussed in Section 2.3, we conclude here that like-ion dispersion should not be included. Considering the slightly more accurate results and better trends in parameter of Full-3 and -4 compared to Full-1 and -2 (r^{MSA} of the salts, as shown in the Supplementary Material), we recommend including like-ion dispersion in the full strategies.

Table 4. Percentage average absolute deviations (AADs) and percentage maximum absolute deviations (MADs) of the salt-specific strategies for the 4 aqueous electrolyte solutions. Deviations larger than 10% are marked as bold and italic.

	MIAC		VLE *p*		Density	
	AAD (%)	MAD (%)	AAD (%)	MAD (%)	AAD (%)	MAD (%)
NaCl						
Disp-1	1.3	6.6	1.1	2.9	0.36	2.1
Disp-2	1.3	6.3	1.1	2.9	0.34	2.1
Disp-3	1.3	7.7	1.2	3.4	0.80	3.9
Disp-4	1.2	7.0	1.2	3.2	0.46	2.7
Assoc-1	0.62	4.4	1.1	2.4	0.32	2.2
Assoc-2	0.76	4.3	1.2	2.5	0.33	2.2
Full-1	0.81	5.4	1.1	2.5	0.69	4.2
Full-2	1.2	5.7	1.1	2.8	0.31	2.1
Full-3	0.57	4.3	1.1	2.2	0.37	2.4
Full-4	0.5	3.6	1.2	2.3	0.37	2.3
KCl						
Disp-1	1.2	4.4	1.5	3.3	0.26	1.3
Disp-2	1.1	3.8	1.5	3.3	0.27	1.3
Assoc-1	0.96	2.5	1.6	3.3	0.30	1.3
Assoc-2	0.42	2.0	1.6	3.3	0.23	1.6
Full-1	0.29	0.58	1.6	3.3	0.27	1.3
Full-2	0.24	0.84	1.6	3.3	0.30	1.5
Full-3	0.88	1.8	1.6	4.2	0.30	1.4
Full-4	0.39	1.6	1.7	3.5	0.29	1.4
RbCl						
Disp-1	0.59	2.6	1.5	6.9	0.27	1.4
Disp-2	0.73	2.0	1.4	7.0	0.44	2.3
Assoc-1	0.42	0.66	1.1	4.3	0.16	0.54
Assoc-2	0.37	0.93	1.1	4.2	0.29	1.0
Full-1	0.56	0.89	1.3	5.4	0.39	2.1
Full-2	1.5	4.2	1.1	2.3	2.4	***11***
Full-3	0.37	1.1	1.1	4.7	0.21	0.79
Full-4	0.51	0.95	1.2	5.8	0.62	2.9
CsCl						
Disp-1	1.8	3.2	2.7	***14***	0.71	3.5
Disp-2	2.1	3.3	2.6	***15***	0.24	1.3
Assoc-1	0.86	3.7	0.94	3.7	0.47	5.0

	MIAC		VLE p		Density	
	AAD (%)	MAD (%)	AAD (%)	MAD (%)	AAD (%)	MAD (%)
Assoc-2	1.1	4.7	1.1	6.0	0.61	4.1
Full-1	0.50	0.95	1.4	7.2	0.29	2.2
Full-2	0.73	2.3	1.5	6.9	0.32	3.2
Full-3	1.5	5.4	1.2	6.7	0.35	2.6
Full-4	1.1	5.4	1.6	5.7	0.40	2.2

The strategies using RPM-1 and -2 present only marginal difference in accuracy.

Figure 4 shows the deviations of the MIAC, VLE and density calculated with Assoc-1 from the experimental data. For references of the experimental data, please see Section 2.2. Results for the other association and full strategies are similar. For MIAC, the data are all at 0.1 MPa. Thus, the deviation of MIAC plotted against p is not shown. In general, the model agrees very well with experimental data over the entire temperature, pressure, and composition range. For the 3 properties, the model is most accurate near 300 K, in which region the data are more extensive. As temperature decreases, deviations increase slightly. Considering that the deviation is at very small x_{ion} at low temperatures, it is much more pronounced compared to that of approximately the same magnitude at much larger x_{ion} at high temperatures. For NaCl, MIAC deviation clearly present a temperature-dependent behavior. Details will be discussed in Section 4.2. Density data are available for the aqueous NaCl and KCl solutions at high temperature; deviations increase very slightly as pressure increases, a large part of which is attributed to the increased deviation of the model for pure water density at higher pressure. Density data are available in the databases up to very high salt composition (close to $x_{\mathrm{ion}} = 0.2$) for the aqueous CsCl solution; deviations increase to approximately 5% at high salt composition, in which range MIAC and VLE data are not available in the database.

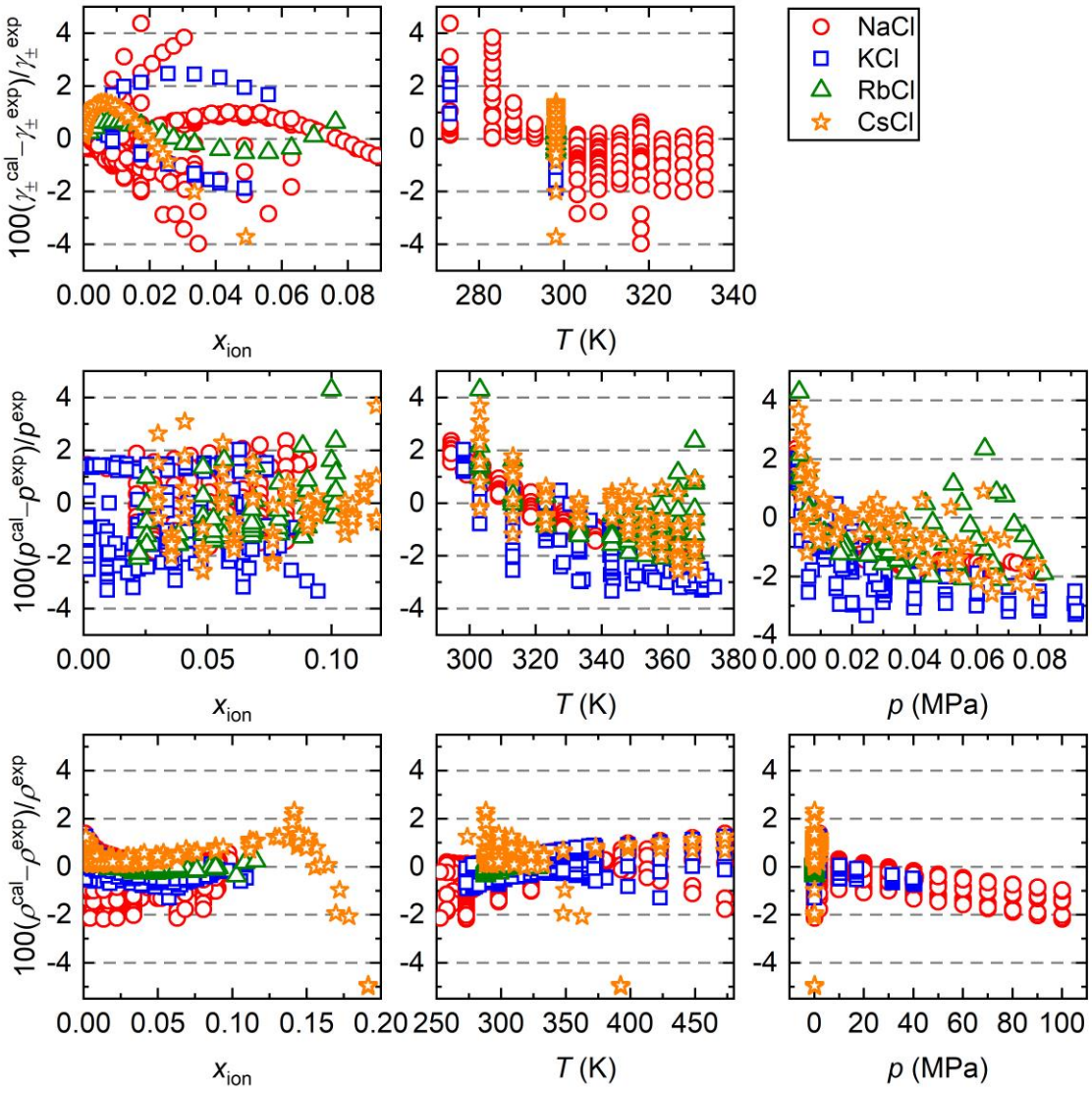

Figure 5. Deviations of the MIAC, VLE and density calculated with Assoc-1 from the experimental data. For references of the experimental data, please see Section 2.2.

3.2 Salt-specific vs. ion-specific parameterization

The AADs and MADs of the ion-specific parameter sets for MIAC, VLE, and density are shown in Table 5. Deviations larger than 10% are marked as bold and italic. Comparing the results in Tables 4 and 5, we can see that the Assoc-I-15 and Assoc-I-12 strategies are as accurate as the salt-specific parameter sets. This is achieved with a much smaller parameter set: 15 or 12 parameters for the 4 salts as compared to 7 for each one of the 4 salts. However, unlike the association strategies, the dispersion and full strategies are not as accurate as the corresponding salt-specific strategies. Large deviations in the VLE of the aqueous CsCl solution are observed for Disp-I-15, Disp-I-12, Full-I-15, and Full-I-12. The only full strategy that achieved comparable accuracy as the association strategies includes 20 parameters (Full-I-20). In the following text, Assoc-I-15 is discussed as an example. Results calculated using

Assoc-I-12 are as accurate for all the properties, except for the density of the aqueous CsCl solution, which has an MAD of 4.2% (still quite good) compared to the MIAC of 2.4% of Assoc-I-15.

Table 5. AADs and MADs of MIAC, VLE, and density of the 4 aqueous alkali halide solutions calculated using the ion-specific strategies. Deviations larger than 10% are marked as bold and italic.

	MIAC		VLE *p*		Density	
	AAD (%)	MAD (%)	AAD (%)	MAD (%)	AAD (%)	MAD (%)
NaCl						
Disp-I-15	1.6	6.4	1.1	2.8	0.62	3.3
Disp-I-12	1.6	6.6	1.1	2.9	0.79	4.0
Assoc-I-15	0.84	5.4	1.1	2.1	0.64	3.4
Assoc-I-12	1.0	5.5	1.1	2.1	0.57	3.2
Full-I-15	1.4	5.8	1.1	2.4	0.72	3.8
Full-I-12	2.2	***10***	1.2	4.0	0.38	2.6
Full-I-20	0.76	4.6	1.1	2.3	0.74	4.2
KCl						
Disp-I-15	1.3	4.6	1.5	3.3	0.25	1.3
Disp-I-12	1.4	4.5	1.5	3.3	0.26	1.3
Assoc-I-15	1.2	4.0	1.6	3.5	0.39	2.0
Assoc-I-12	1.3	3.0	1.5	3.3	0.32	1.6
Full-I-15	1.3	4.4	1.5	3.3	0.32	1.3
Full-I-12	2.8	7.7	1.4	3.3	0.43	2.6
Full-I-20	1.1	3.6	1.5	3.3	0.32	1.4
RbCl						
Disp-I-15	0.64	1.7	1.4	6.8	0.20	1.0
Disp-I-12	0.68	1.9	1.4	6.9	0.20	0.96
Assoc-I-15	0.54	1.2	1.1	4.1	0.20	1.3
Assoc-I-12	0.64	1.1	1.1	3.8	0.25	1.6
Full-I-15	0.51	1.3	1.3	6.4	0.18	0.68
Full-I-12	1.8	4.4	1.4	7.5	0.26	1.6
Full-I-20	0.75	1.2	1.2	3.9	0.20	0.94
CsCl						
Disp-I-15	1.8	3.1	2.7	***14***	0.89	4.1
Disp-I-12	1.8	3.1	2.6	***14***	0.82	3.8
Assoc-I-15	1.5	6.5	1.2	5.5	0.42	2.4
Assoc-I-12	1.1	5.4	1.3	5.2	0.65	4.2
Full-I-15	1.8	2.8	2.4	***14***	0.36	2.4
Full-I-12	3.0	6.0	1.9	***11***	0.70	4.4
Full-I-20	1.3	4.5	1.1	5.1	0.58	3.4

Figures 6 and 7 show the comparison of the MIAC and density of the aqueous NaCl, KCl, RbCl, and CsCl solutions calculated using Assoc-I-15 and experimental data at 298.15 and 0.1

MPa. The experimental data are from Ref [52,57,70,107,161,242]. The model is very accurate at atmospheric conditions. Figure 8 shows the comparison of density of aqueous NaCl and KCl solutions calculated using Assoc-I-15 and experimental data at 298.15 K and elevated pressure, up to 100 MPa for NaCl and 40 MPa for KCl. The experimental data are from Ref [112,145]. The deviations are slightly larger than at 0.1 MPa, and increase with increasing pressure and salt composition, but are within 2%. At higher pressure, the deviations for pure water of the PPC-SAFT model is also slightly larger, as shown in the left side of the graphs (at 0 salt composition). For the aqueous RbCl and CsCl solutions, data are not available up to such high pressure. Figure 9 shows the vapor pressure of aqueous KCl solution calculated using Assoc-I-15 and experimental data at 313.15 to 343.15 K. The experimental data are from Ref [88]. Results are similar for the other aqueous electrolyte solutions. Overall, the properties are correlated very accurately.

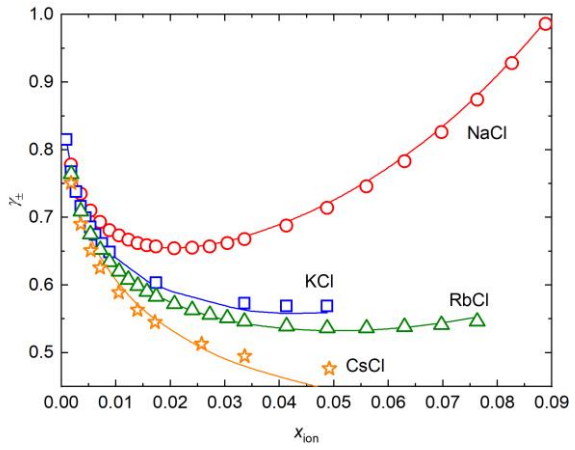

Figure 6. Comparison of the MIAC of the aqueous NaCl, KCl, RbCl, and CsCl solutions calculated using Assoc-I-15 and experimental data at 298.15 K and 0.1 MPa. The experimental data are from Ref [52,57,70].

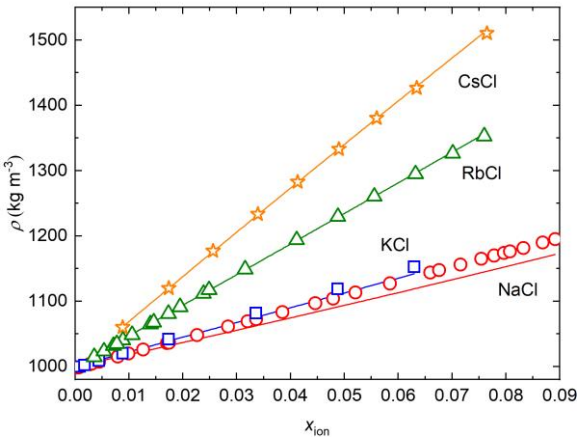

Figure 7. Comparison of the density of the aqueous NaCl, KCl, RbCl, and CsCl solutions calculated using Assoc-I-15 and experimental data at 298.15 K and 0.1 MPa. The experimental data are from Ref [107,161,242].

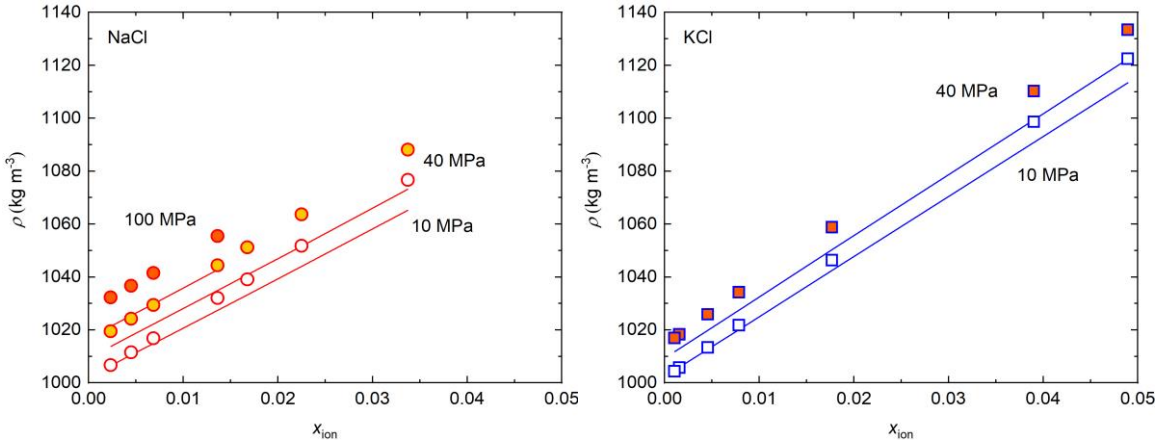

Figure 8. Comparisons of the density of the aqueous NaCl and KCl solutions calculated using Assoc-I-15 and experimental data at 298.15 K and elevated pressures. The experimental data are from Ref [112,145].

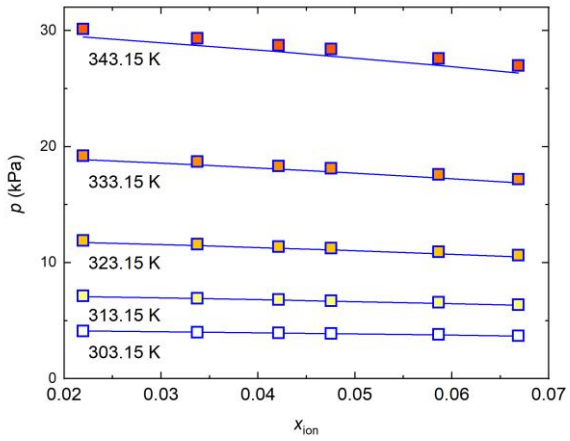

Figure 9. Comparison of the vapor pressure of the aqueous KCl solution calculated using Assoc-I-15 and experimental data at 313.15 to 343.15 K. The experimental data are from Ref [88].

4 Discussion

In this section, the contributions of the terms are analyzed; the model is tested on the MIAC over large temperature ranges beyond the range of the data used in the regression. The model is also tested on the osmotic coefficient and individual ion activity coefficient, which have not been included in the parameter estimation.

4.1 Contributions of the terms

Figure 10 shows the contributions to $\ln \gamma_{\pm}$ of the terms (hard-chain, dispersion, association, multipolar, MSA, and Born) in the ion-specific strategies, Assoc-I-15, Disp-I-15, and Full-I-15, at 298.15 K and 0.1 MPa. The reference state of the sum of $\ln \gamma_{\pm}$ is naturally based on the molar fraction unit. The contributions of Assoc-I-12, Disp-I-12, Full-I-12, and Full-I-20 are similar to the corresponding 15-parameter cases, and are not shown here. At low salt composition, $\ln \gamma_{\pm}$ is dominated by the MSA term. The MSA term presents a curvature,

while all the other terms are close to linear in the entire ranges, counter-balancing the negative MSA term. Thus, $\ln \gamma_{\pm}$ presents an upward curvature as salt composition increases. The Born term is approximately the same in the different strategies for each aqueous electrolyte solution, because it is determined by the relative permittivity and hard sphere diameters. The multipolar term presents a very small contribution, indicating that our conclusions would also apply for a SAFT model that does not include a multipolar term. The contributions of the salt-specific parameterization strategies are provided in the Supplementary Material. The behavior is very similar for the ion- and salt-specific association strategies, and is different for the dispersion and full strategies. This could be linked to the observation that reducing the number of adjustable parameters does not have a considerable impact on the accuracy of the model for the association strategies.

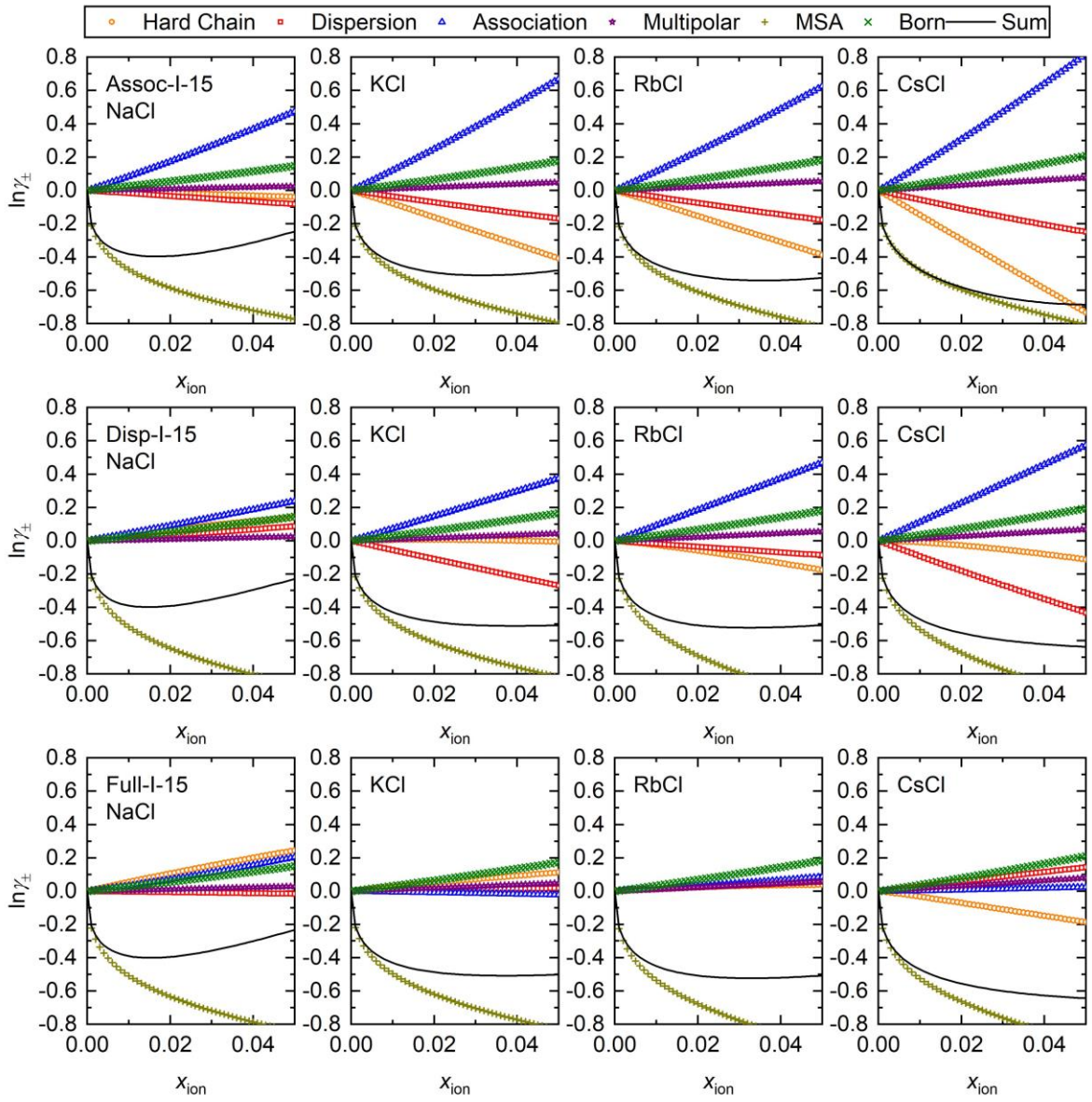

Figure 10. Contributions to $\ln \gamma_{\pm}$ of the terms in the ion-specific strategies, Assoc-I-15, Disp-I-15, and Full-I-15, at 298.15 K and 0.1 MPa.

For Assoc-I-15, the association term presents the largest positive contribution for the 4 aqueous electrolyte solutions, while the dispersion and hard chain terms are negative and quite pronounced. Note that, in the association strategies, the dispersion contribution is a consequence of only the water-water dispersion interaction. The segment number is set at 1 for the ions. The regressed segment number for water is also close to 1. Therefore, the hard chain contribution is approximately a hard sphere contribution.

For Disp-0I-15, the association term also presents the largest positive contribution, but is smaller compared to the Assoc-I-15 cases. Note that, in the dispersion strategies, the association contribution is a consequence of only the water-water association interaction. The

hard chain and dispersion terms are positive for the aqueous NaCl solution, and are smaller (in magnitude, negative) for the other aqueous solutions compared to the Assoc-I-15 cases.

For Full-I-15, the association contribution is even smaller compared to the dispersion cases. The association, hard chain, and dispersion terms present no trend. Considering that these strategies resulted in no improvement in accuracy compared to the association strategies, the counter-balancing behavior of the close-to-linear terms shows that there is no need to account for both the association and dispersion contributions for the short-range ion-ion and ion-solvent interactions.

Naturally, the total $\ln \gamma_{\pm}$ is of course approximately the same for the different strategies for each salt. However, it is also interesting to notice that the magnitudes of the separate contributions are larger for salts with heavier cations for the association and dispersion strategies.

In the ePPC-SAFT model, the electrolyte contribution (MSA and Born) and the "physical" contributions (that are all approximately linear) balance each other out.; Yet, the distribution among the physical terms is sometimes very different, with, for example, sometimes positive, sometimes negative contributions from the dispersion and hard sphere. The association strategies show a logical trend when increasing the cation size in contrast to the other strategies. At this point, we don't have a sufficiently clear vision of the true physics to comment on the meaning of these contrasting contributions, but the trend observed with the association strategy provides better ground for further work.

4.2 Temperature dependence of MIAC

Figure 11 shows the comparison of the MIAC of the aqueous NaCl solution calculated using Assoc-1 and experimental data from 273.15 to 383.15 K. The data used for comparison are from Ref [303], and are not used in the regression. It covers larger temperature range than the MIAC data used in the regression, which are only up to 333.15 K, and also covers larger salt composition range at low temperatures. MIAC presents an anomaly: at low temperatures, MIAC increases with increasing temperature. Figure 12 shows results calculated using the ion-specific strategy, Assoc-I-15. Neither parameter set captures the temperature-dependence anomaly. As temperature increases above the range of the data used in the regression, the salt-specific parameter set, Assoc-1, agrees with experimental data very well, while the ion-specific parameter set, Assoc-I-15, presents slightly larger deviations.

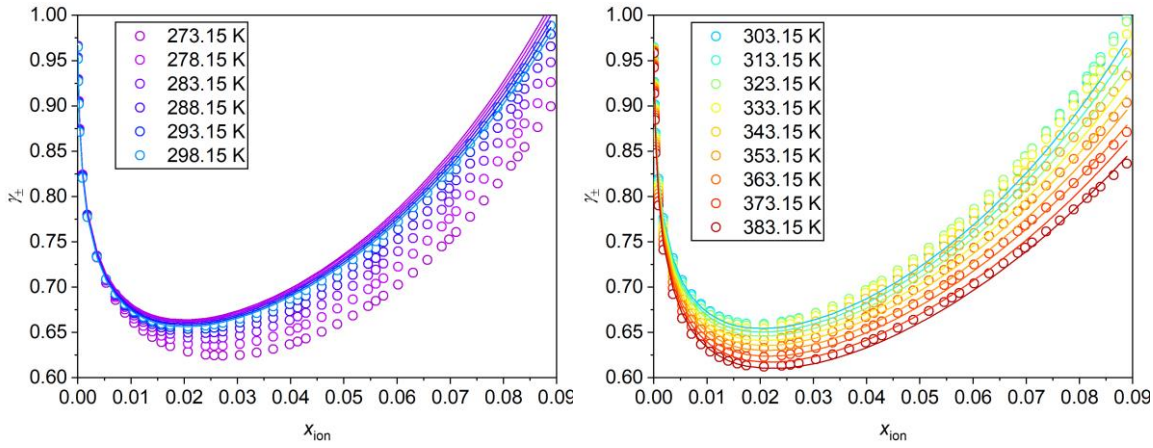

Figure 11. Comparison of the MIAC of the aqueous NaCl solution calculated using Assoc-1 and experimental data from 273.15 to 383.15 K.

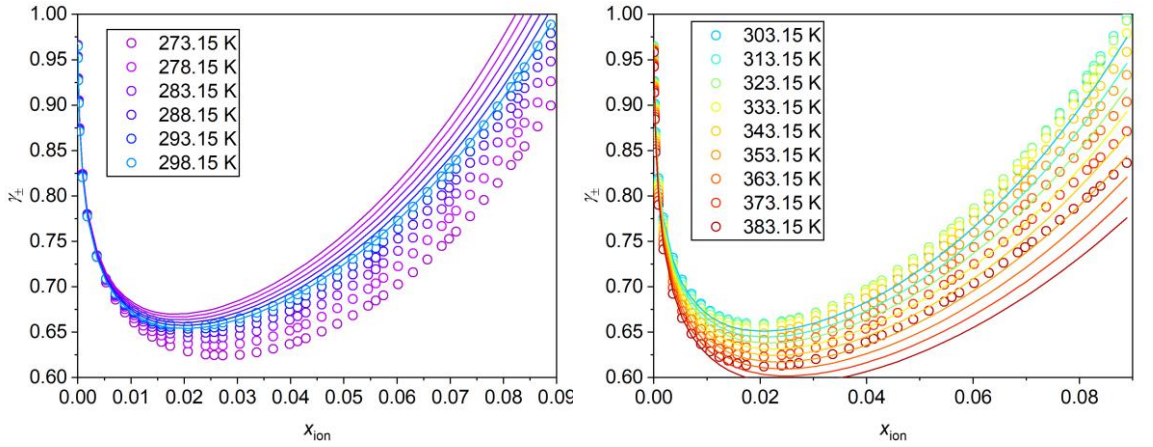

Figure 12. Comparison of the MIAC of the aqueous NaCl solution calculated using Assoc-I-15 and experimental data from 273.15 to 383.15 K.

Efforts have been made in the literature to capture the temperature-anomaly of MIAC. Selam et al. [44] captured the temperature-anomaly using temperature-dependent dispersion energy parameters. Roa Pinto et al. [40] captured the temperature-dependence anomaly without introducing temperature-dependent interaction energy parameters. Specifically, the only parameter set that managed to capture the temperature-dependence is the 10-parameter association strategy, "model 2.0". However, the regressed MSA diameter was smaller than the HS diameter for Cl^-. Difference between the parameterization strategies of this work and Ref [40] are:

- The parameter sets are different. In Ref [40], there are more adjustable parameters, e.g., an extra binary interaction parameter was included for association volume.
- Ionic diameters were not forced to meet the physical consistency constraints in Ref [40]. The regressed anion MSA diameter was smaller than the HS diameter. In this work, the ionic diameters consistency is enforced in the regression.

- The included data are different. In Ref [40], representative datasets were used, covering larger ranges quite evenly. On the other hand, in this work, experimental data from extensively collected and evaluated databases are used. The availability of such data inevitably favors the ranges near room temperature (298.15 K).
- More importantly, enthalpy data was included in the objective function of Ref [40]. The property, although only qualitatively represented, could be significantly important for the temperature dependence of the MIAC.

Here we refrain from using enthalpy data for the following reasons:

- In future works, the model will be extended to mixed-solvent electrolyte solutions, for which enthalpy data are very scarce.
- The model has been shown to present large deviations from the experimental enthalpy data in Ref [40]. The best that could be achieved was a qualitative agreement. Including the data would jeopardize the highly accurate representation of the MIAC, VLE, and density data in this work.

Enforcing the ionic diameter consistency in the regression, efforts are made to obtain the same temperature dependence as in Ref [40]. When regressed to the evenly distributed pseudo-experimental MIAC dataset from Ref [303], the obtained parameter set captures a maximum, as shown in Figure 13. Only MIAC is included in this regression. This parameterization strategy is here noted as Assoc-MIAC. When VLE and density data are also included in the objective function along with the evenly distributed MIAC dataset, a maximum in MIAC is also captured, however, the isotherms are rather close to each other; the temperature-dependence is not captured as well as when using Asso-MIAC. In principle, the joint effect of the decreasing Wertheim association term and increasing other terms can capture the maximum of MIAC with temperature. However, whether it is captured is a matter of parameter regression. The use of an extra binary interaction parameter for the association volume has been found to result in only marginal difference. The parameters are provided in the Supplementary Material, along with the comparisons of this parameter set and the Ref [40] with the data summarized in Table 1 for the aqueous NaCl solution. Figure 14 shows a comparison of the MIAC temperature-dependence of the modeling strategies Assoc-1, Assoc-I-15, Assoc-MIAC, and Assoc-R40 (the parameter set from Ref [40]) at 2, 4, and 6 M from 273.15 to 383.15 K. Assoc-MIAC and Assoc-R40 correctly represent the temperature dependence of MIAC, while Assoc-1 and Assoc-15 present monotonically decreasing trends with temperature.

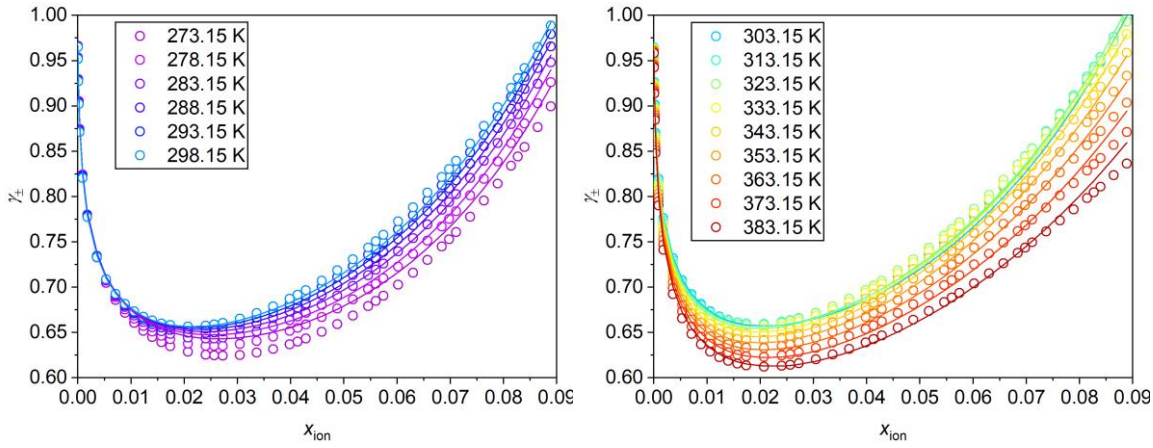

Figure 13. Comparison of the MIAC of the aqueous NaCl solution calculated using Assoc-MIAC and experimental data from 273.15 to 383.15 K.

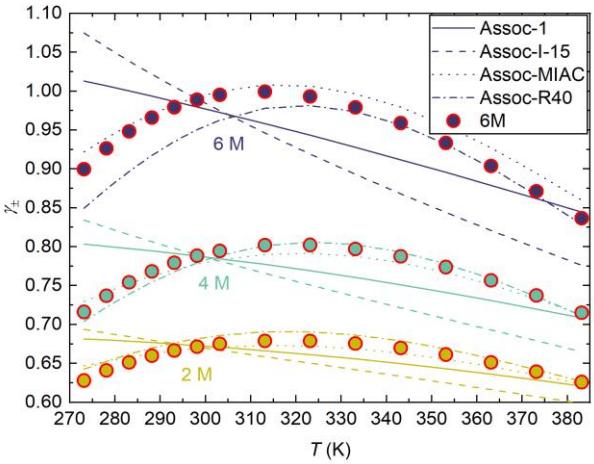

Figure 14. Comparison of the MIAC temperature-dependence of the modeling strategies Assoc-1, Assoc-I-15, Assoc-MIAC, and Assoc-R40 at 2, 4, and 6 M from 273.15 to 383.15 K.

An advantage of the salt- and ion-specific parameter sets in this work (Asso-1 and Asso-I-15), compared to Asso-MIAC and Asso-R40, is that they are more accurate close to 298.15 K, which is the region where most data are located, especially considering that the model is to be extended to mixed-solvent electrolyte solutions. Therefore, the temperature-anomaly at low temperature has not been further pursued in this work.

4.3 Osmotic coefficient

The model is tested on the osmotic coefficient, which is not included in the parameter estimation. The osmotic coefficient is related to the MIAC according to the Gibbs-Duhem equation. Therefore, if the MIAC is accurately represented with the model, the osmotic coefficient is also expected to be accurately predicted. Therefore, the TherefoirExperimental osmotic coefficient data have been evaluated in Ref [7]. Because MIAC and VLE data are up to 400 K in the regression, osmotic coefficient data above 400 K are removed in our study. Furthermore, the osmotic coefficient data of the aqueous RbCl and CsCl solutions from Ref [7]

cover a much larger salt composition range compared to the MIAC data used in the regression. Therefore, the salt composition is limited to 6 M in this section (approximately $x_{\mathrm{ion}} = 0.089$, close to the solubility of NaCl in water at 298.15 K). For the aqueous KCl, RbCl, and CsCl solutions, the range is larger than the MIAC data range (as shown in Table 1).

Table 6 shows the osmotic coefficient data and prediction deviations of the ion-specific parameter set, Assoc-I-15. Figure 15 shows the comparison of the osmotic coefficient of aqueous NaCl, KCl, RbCl, and CsCl solutions calculated using Assoc-I-15 and experimental data at 298.15 K and 0.1 MPa. Please note the very small scale in the graph. Overall, the model predicts the osmotic coefficient very well. For the aqueous NaCl solution, the calculated curve is in good agreement with the experimental data. For the aqueous KCl and RbCl solutions, deviations increase very slightly as salt composition exceeds the range of the MIAC data that are used in the regression; maximum deviations are within 5%. For the aqueous CsCl solution, deviation increases to more than 6% at approximately $x_{\mathrm{ion}} = 0.05$. As shown in Table 1, CsCl MIAC data are available only up to $x_{\mathrm{ion}} = 0.049$ for the mixture. Furthermore, the MIAC deviation is more than 4% at $x_{\mathrm{ion}} = 0.049$ (as shown in Figure 6), in which range the largest osmotic coefficient deviation is located. Above the MIAC data range and up to $x_{\mathrm{ion}} = 0.089$, the osmotic coefficient deviation decreases. However, outside of the range of the comparisons here, the osmotic coefficient data are available up to very high composition. The more drastic increase of the model compared to the experimental data retains as composition increases above what is shown in Figure 16, with the osmotic coefficient being 1.26 at $x_{\mathrm{ion}} = 0.15$ (larger than 11 M, far beyond the MIAC data range), where the experimental osmotic coefficient is 1.02.

Table 6. Osmotic coefficient data and prediction deviations of the ion-specific parameter set, Assoc-I-15.

Wate +	T (K)	p (MPa)	x_{ion}	N_{dp}	References	AAD (%)	MAD (%)
NaCl	298.15 ~ 398.15	0.1 ~ 0.4	~ 0.089	73	[304–306]	1.6	3.5
KCl	273.15 ~ 372.75	0.1 ~ 0.2	~ 0.079	95	[74,307–310]	1.4	4.7
RbCl	298.15	0.1	~ 0.089	32	[304,311]	0.82	4.2
CsCl	298.15 ~ 383.15	0.1	~ 0.089	35	[60,312]	2.8	6.6

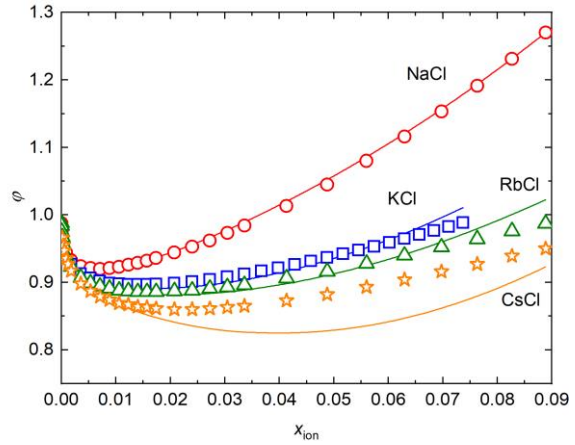

Figure 15. Comparison of the osmotic coefficient of the aqueous NaCl, KCl, RbCl, and CsCl solutions calculated using Assoc-I-15 and experimental data at 298.15 K and 0.1 MPa.

Figure 16 shows the comparison of the osmotic coefficient of the aqueous NaCl solutions calculated using Assoc-I-15 and experimental data from 298.15 to 398.15 K. Unlike for the MIAC, experimental data are not available for the osmotic coefficient at lower temperatures. An overlap is observed in the experimental data at 298.15, 318.15, and 333.15 K, indicating that there is an osmotic coefficient maximum in the temperature range. The ion-specific parameter set predicts a monotonic decrease with temperature, like for the MIAC, and fails to capture the temperature maximum. Furthermore, the deviation is slightly larger at elevated temperatures. The salt-specific parameter sets, Assoc-1, Assoc-MIAC, and Assoc-R40, capture the high temperature behavior better than Assoc-I-15.

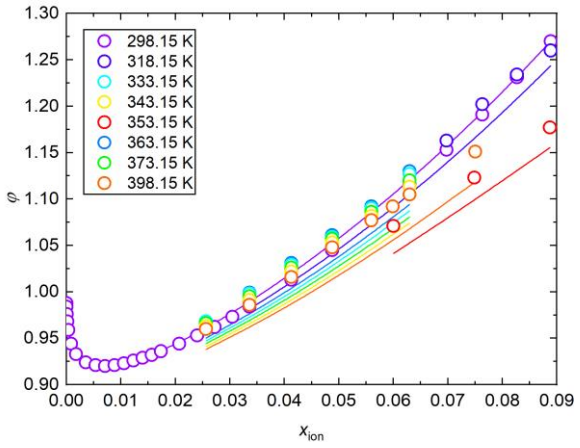

Figure 16. Comparison of the osmotic coefficient of the aqueous NaCl solutions calculated using Assoc-I-15 and experimental data from 298.15 to 398.15 K.

4.4 Individual ion activity coefficient (IIAC)

In addition to the mean properties, IIAC is an important property that can be used for further testing the model. IIAC is important in that it appears in the Nernst equation for the electrode potential in a half-cell [313]. In the ion-specific parameterizations, the 4 aqueous

alkali chloride solutions are regressed together, introducing more information about the individual ions in the regression by the different cations and the common anion, Cl^-.Although there is some debate about the validity of the experimental measurement of the activity coefficient of individual ions [314–320], recent molecular simulations [321] qualitatively agrees with the experimental data. Therefore, IIAC is used as a qualitative test here.

Experimental [322,323] and molecular simulation [321] investigations presented that the relative magnitudes of the cation and anion IIAC for the aqueous NaCl and KCl solutions are opposite. In the salt-specific parameterization in this work, the only individual ion information that are introduced are: the HS diameters, which are proportional to the Pauling diameters, and the Born diameters, which are determined based on the Gibbs energy of solvation. All 10 salt-specific strategies fail to correctly predict the larger IIAC for Na^+. All the properties used in the objective function are mean properties, i.e., individual ion information is not introduced from the data. In the ion-specific parameterizations, the 4 aqueous alkali chloride solutions are regressed together, introducing more information about the individual ions in the regression by the different cations and the common anion, Cl^-.

Figure 17 compares the IIAC of the aqueous NaCl and KCl solutions calculated using the salt-specific strategy, Assoc-1, ion-specific strategies, Assoc-I-15, Disp-I-15, and Full-I-15, and experimental data. The experimental data are from Ref [322,323]. This property is not included in the regression. Thus, these results are pure predictions. Assoc-I-15 correctly predicts the opposite relative magnitudes of the cation and anion IIAC of the aqueous NaCl and KCl solutions, while the other strategies predict smaller IIAC for the cation in both cases. Results are similar for the 12-parameter ion-specific strategies: Assoc-I-12 correctly predicts the opposite relative magnitudes, while Disp-I-12 and Full-I-12 fail. Table 7 summarizes whether the opposite relative magnitudes of the cation and anion IIAC of the aqueous NaCl and KCl solutions is correctly predicted by the ion-specific strategies. In a nutshell, the ion-specific association strategies present an advantage for predicting the qualitative behavior of IIAC over the ion-specific dispersion and full strategies and the salt-specific strategies.

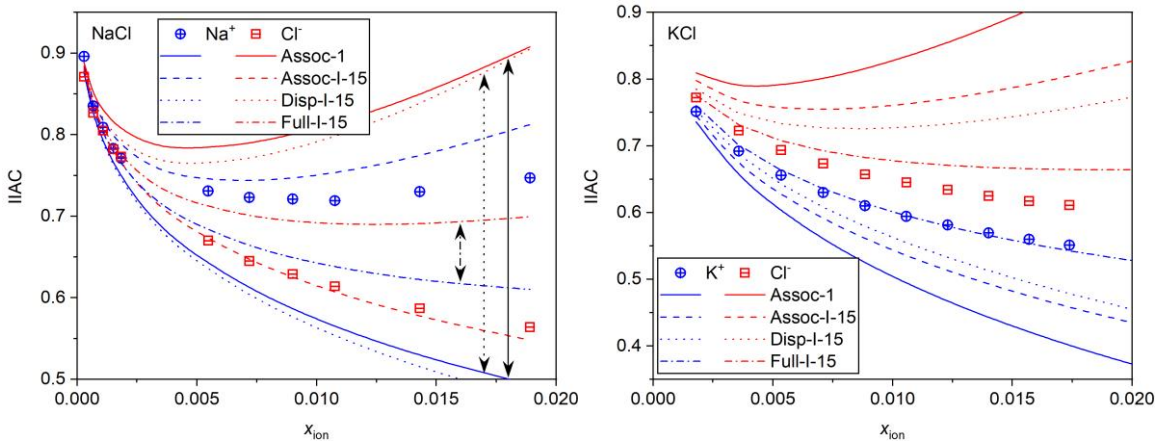

Figure 17. Comparison of the IIAC of the aqueous NaCl and KCl solutions calculated using the salt-specific strategy, Assoc-1, ion-specific strategies, Assoc-I-15, Disp-I-15, and Full-I-15, and experimental data.

Table 7. Whether the opposite relative magnitudes of the cation and anion IIAC of the aqueous NaCl and KCl solutions is correctly predicted by the ion-specific strategies.

Parameterization strategies	Opposite relative magnitudes
Asso-I-15	☺
Asso-I-12	☺
Disp-I-15	☹
Disp-I-12	☹
Full-I-15	☹
Full-I-12	☹
Full-I-20	☹

5 Conclusions

In this work, the ePPC-SAFT model is parameterized in an ion-specific approach enforcing physical consistency of the ionic parameters. Properties that are useful in practical applications are included in the objective function, i.e., MIAC, VLE, and density. Reference data are taken from extensively collected and critically evaluated databases. The association, dispersion, and full (association + dispersion) approaches are compared for the short-range ion-ion and ion-solvent interactions. Efforts are made to parameterize the model in an ion-specific manner with minimum loss of accuracy. The ion-specific parameter sets are compared with the salt-specific sets. The model and parameter sets are further tested on the MIAC beyond the data range of the regression, and on properties that have not been included in the regression. The major conclusions are:

- For the salt-specific cases, all strategies are quite accurate in the entire temperature, pressure, and salt composition range of the experimental database; the association and full strategies are more accurate than the dispersion strategies. Like-ion dispersion should not

be included in the dispersion strategies, but is recommended to be included in the full strategies. Despite using a larger number of adjustable parameters and including more completely the physical interactions, the full strategies are not more accurate than the association strategies. Similar results are obtained both the investigated RPMs.

- For the ion-specific cases, the association strategies are approximately as accurate as the salt-specific cases in terms of the average and maximum deviations, while the dispersion and full strategies are less accurate. To obtain the same accuracy as the association strategies, the full strategy has to use a larger number of adjustable parameters. This may indicate a reason not to include both dispersion and association for the short-range ion-ion and ion-solvent interactions. The 12-parameter ion-specific association strategy with the same binary interaction parameter for the 4 salts is only slightly less accurate than the 15-parameter case.
- However, at higher temperature, the ion-specific association strategy is less accurate than the salt-association association strategy. Neither salt- or ion-specific strategy represent the MIAC temperature maximum of the aqueous NaCl solution, which was successfully represented in the literature, using temperature-dependent energy parameters or a physically inconsistent parameter set. The behavior is successfully represented here using the association approach by regressing only to an evenly distributed pseudo-experimental MIAC dataset. However, the attempt is dropped because the ion-specific association parameter set is more extendable and more accurate overall speaking for all investigated properties, with the temperature-anomaly in MIAC resulting in only slightly larger deviations.
- An analysis of the contributions of the terms shows that the dispersion, association, and hard chain terms are all close to linear with salt composition, and counter-balance each other in all cases. The various terms present no trend within the alkali chloride series in the full strategies. Therefore, the association strategies are possibly more favorable compared to the dispersion and full strategies.
- The model and parameter set is tested on the osmotic coefficient and individual ion activity coefficient, which are not included in the regression. The ion-specific association parameter set accurately represents the osmotic coefficient over wide temperature and salt composition ranges, beyond those of the MIAC data used in the regression. The ion-specific association strategies correctly predict the opposite relative magnitudes of the cation and anion individual ion activity coefficient of the aqueous NaCl and KCl solutions, while the ion-specific dispersion and full strategies, and all the salt-specific strategies fail.

To sum up, state-of-the-art parameter sets have been obtained for the ePPC-SAFT model, facilitating benchmarking of the short-range interaction approaches, and salt- and ion-specific parameterizations. We recommend including the Wertheim association for the short-range ion-ion and ion-solvent interactions, and parameterizing SAFT models in an ion-specific manner using physically consistent parameters. In the future, the model will be extended to other aqueous electrolyte solutions, and mixed-solvent and mixed-salt electrolyte solutions.

CRediT authorship contribution statement

Fufang Yang: Conceptualization, Methodology, Software, Validation, Formal Analysis, Investigation, Data Curation, Writing – Original Draft, Visualization. Tri-Dat Ngo: Software. Juan Sebastian Roa Pinto: Methodology. Georgios M. Kontogeorgis: Conceptualization, Supervision, Writing – Review & Editing, Funding Acquisition. Jean-Charles de Hemptinne: Conceptualization, Resources, Supervision, Software, Writing – Review & Editing, Project Administration, Funding Acquisition.

Declaration of competing interest

The authors declare no competing financial interest.

Acknowledgements

The authors wish to thank the European Research Council (ERC) for funding of this research under European Union's Horizon 2020 research and innovation program (grant agreement No. 832460), ERC Advanced Grant project "New Paradigm in Electrolyte Thermodynamics".

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