

## Retraction

# Retracted: Modeling of Vapor-Liquid Equilibrium for Electrolyte Solutions Based on COSMO-RS Interaction

### Journal of Chemistry

Received 23 January 2024; Accepted 23 January 2024; Published 24 January 2024

Copyright © 2024 Journal of Chemistry. This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

This article has been retracted by Hindawi following an investigation undertaken by the publisher [1]. This investigation has uncovered evidence of one or more of the following indicators of systematic manipulation of the publication process:

- (1) Discrepancies in scope
- (2) Discrepancies in the description of the research reported
- (3) Discrepancies between the availability of data and the research described
- (4) Inappropriate citations
- (5) Incoherent, meaningless and/or irrelevant content included in the article
- (6) Manipulated or compromised peer review

The presence of these indicators undermines our confidence in the integrity of the article's content and we cannot, therefore, vouch for its reliability. Please note that this notice is intended solely to alert readers that the content of this article is unreliable. We have not investigated whether authors were aware of or involved in the systematic manipulation of the publication process.

Wiley and Hindawi regrets that the usual quality checks did not identify these issues before publication and have since put additional measures in place to safeguard research integrity.

We wish to credit our own Research Integrity and Research Publishing teams and anonymous and named external researchers and research integrity experts for contributing to this investigation.

The corresponding author, as the representative of all authors, has been given the opportunity to register their agreement or disagreement to this retraction. We have kept a record of any response received.

### References

- [1] W. Liu, C. Zhao, Y. Zhou, and X. Xu, "Modeling of Vapor-Liquid Equilibrium for Electrolyte Solutions Based on COSMO-RS Interaction," *Journal of Chemistry*, vol. 2022, Article ID 9070055, 13 pages, 2022.

## Research Article

# Modeling of Vapor-Liquid Equilibrium for Electrolyte Solutions Based on COSMO-RS Interaction

Weiping Liu,<sup>1</sup> Chun Zhao,<sup>2,3</sup> Yu Zhou,<sup>1</sup> and Xianzhen Xu <sup>1,3</sup>

<sup>1</sup>College of Chemistry and Chemical Engineering, Instrumental Analysis Center of Qingdao University, Shandong Sino-Japanese Center for Collaborative Research of Carbon Nanomaterials, Collaborative Innovation Center for Marine Biomass Fiber Materials and Textiles, Laboratory of Fiber Materials and Modern Textile, Qingdao University, Qingdao 266071, Shandong, China

<sup>2</sup>Qingdao Hengxing University of Science and Technology, Qingdao 266100, China

<sup>3</sup>Qingdao Boting Hydrogen Age Ocean Technology R&D Center, Qingdao Boting Technology Co., Ltd, Qingdao 266100, Shandong, China

Correspondence should be addressed to Xianzhen Xu; [xuxianzhen@qdu.edu.cn](mailto:xuxianzhen@qdu.edu.cn)

Received 29 July 2022; Revised 19 August 2022; Accepted 23 August 2022; Published 29 September 2022

Academic Editor: Ajay Rakkesh R

Copyright © 2022 Weiping Liu et al. This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

The modeling of phase equilibrium for electrolyte solutions plays an important role in chemical thermodynamics. Modeling and calculation of the vapor-liquid equilibrium (VLE) for an electrolyte solution are studied in this paper. The influence mechanism for the microscopic interaction on the macroscopic VLE is further studied by COSMOtherm. Then, a developed model is proposed. The interaction parameters in the model are linked to the COSMO interaction energy ( $H_{int}$ ). The interaction equations are remodeled using 1stopt software, and components are used to replace the “interaction parameters” used in a previous model. The developed model can be used to successfully predict VLE data for electrolyte solutions based on the  $\alpha$  and  $h_i$  parameters.

## 1. Introduction

Simulation calculations of the phase equilibrium for electrolyte solutions play an important role in industrial and natural processes. Thermodynamic models are widely used in vapor-liquid equilibrium (VLE), solid-liquid equilibrium (SLE), and liquid-liquid equilibrium calculations. The most used thermodynamic model is the activity coefficient model. Therefore, the study of the activity coefficient model is traditional research, but it is more significant.

Since the proposal of Debye-Hückel's law [1] for a strong electrolyte solution, a number of models have been developed, including physical, chemical, and local composition models [2]. In the physical model, physical interactions have been used to describe the deviation from Debye-Hückel's law, for example, the Pitzer model [3] and the modified Pitzer model [4, 5]. In the chemical model, chemical reactions have been used to describe the properties of electrolyte

solutions: the Robinson and Stokes model [6] and the Lu-Maurer model [7]. The local composition models combine the short-range interactions (Wilson [8], NRTL [9], and UNIQUAC [10]) with the long-range interactions (Debye-Hückel's law or modified Debye-Hückel's law [1]). Some examples are the ElecNRTL model [11, 12], the OLI MSE model [13], and Thomsen's model [14]. In addition, many models have been developed and evolved on the basis of the above models, such as the LIQUAC model [15], Xu's model [16], the PSC model [17], the PC-SALT model [18], and so on. As the coefficient models have evolved, there has been great progress in the scope of application and calculation accuracy. Iwai et al. conducted research on simultaneous correlation of liquid-liquid equilibria of ternary systems and phase equilibria of constituent binary systems using an improved new activity coefficient model [19]. Noumir et al. conducted research on isobaric vapor-liquid equilibrium data modeling of ternary systems containing

ionic liquids [20]. However, there are increased limitations in the interpretation of interactions, which represent the bottleneck problem for thermodynamic model research.

In the study of thermodynamic models for electrolyte solutions, many scholars have realized the importance of microinteractions for thermodynamic research. Pitzer [3] recognized the correlation between the interaction between ions and ionic strength and established a more widely used activity coefficient model. Chen [11, 12] considered the contribution of ion electrostatic interactions and improved the local composition model. In addition, many activity coefficient models [21–23] have been established on the basis of the interaction hypothesis. Some scholars have studied the activity coefficient and interaction in thermodynamics using COSMO [24–26]. However, due to the limitation of the experimental conditions at the time, many microscopic interaction concepts are only used for the construction of electrolyte solution models, lacking quantification of the interaction and the structure-activity relationship with the phase balance properties. These are also the main research directions of this paper.

## 2. The Extended NRTL Model

In this part, the modified NRTL model proposed by Xu et al. [27, 28] was used. The model was applied to calculate the VLE data for mixed electrolyte solutions over wide ranges of temperature and molarity. Based on previous works [27, 28], the impact mechanism of microscopic interactions on macroscopic VLE was further investigated. The thermodynamic activity coefficient model is described as follows:

$$\% \frac{n_i G_{NRTL}^e}{RT} = m_x m_w \left( \frac{\tau_{w,x} G_{w,x}}{m_x + m_w G_{w,x}} + \frac{\tau_{x,w} G_{x,w}}{m_w + m_x G_{x,w}} \right), \quad (1)$$

$$G_{w,x} = \exp(-\alpha \tau_{w,x}), \quad (2)$$

$$G_{x,w} = \exp(-\alpha \tau_{x,w}), \quad (3)$$

where  $G_{NRTL}^e$  is the excess Gibbs energy equation of NRTL,  $n_t$  is the total molar,  $m_x$  is the total molality of solute, and  $\alpha$  is the randomness parameter.

$$m_w = \frac{1000}{Ms} - \sum_{i=1}^n (h_i m_i), \quad (4)$$

where  $h_i$  is the hydration parameter and  $Ms = 18.0152$ .

$$\tau_{w,x} = \frac{\sum_{i=1}^n (\tau_{w,i} m_i)}{\sum_{i=1}^n (m_i)}, \quad (5)$$

$$\tau_{x,w} = \frac{\sum_{i=1}^n (\tau_{i,w} m_i)}{\sum_{i=1}^n (m_i)}, \quad (6)$$

$$\tau_{w,i} = \frac{\tau_{w,i}^{(0)} + \tau_{w,i}^{(1)}}{T}, \quad (7)$$

$$\tau_{i,w} = \frac{\tau_{i,w}^{(0)} + \tau_{i,w}^{(1)}}{T}, \quad (8)$$

where  $\tau_{w,x}$ ,  $\tau_{x,w}$  and  $\tau_{w,i}$ ,  $\tau_{i,w}$  are water-solute action terms and solute-water action terms.  $\tau_{w,i}$  and  $\tau_{i,w}$  are the temperature parameters.

In the COSMO calculation process, equations (5) to (8) are very unsatisfactory for the description of the interaction. The new interaction equation is expressed as follows:

$$\tau_{w,x} = \sum_{i=1}^n (\tau_{w,i}^a \exp(\tau_{w,i}^b m_i) + \tau_{w,i}^c \exp(\tau_{w,i}^d m_i)), \quad (9)$$

$$\tau_{x,w} = \sum_{i=1}^n (\tau_{i,w}^a \exp(\tau_{i,w}^b m_i) + \tau_{i,w}^c \exp(\tau_{i,w}^d m_i)), \quad (10)$$

$$\tau_{w,i}^x = \frac{\tau_{w,i}^{(x-0)} + \tau_{w,i}^{(x-1)}}{T + \tau_{w,i}^{(x-2)} \ln(T)}, \quad (11)$$

$$\tau_{i,w}^x = \frac{\tau_{i,w}^{(x-0)} + \tau_{i,w}^{(x-1)}}{T + \tau_{i,w}^{(x-2)} \ln(T)}, \quad (12)$$

where  $\tau_{w,x}$  and  $\tau_{x,w}$  are water-solute action terms and solute-water action terms.  $\tau_{w,i}^a$ ,  $\tau_{w,i}^b$ ,  $\tau_{w,i}^c$ ,  $\tau_{w,i}^d$ ,  $\tau_{i,w}^a$ ,  $\tau_{i,w}^b$ ,  $\tau_{i,w}^c$ , and  $\tau_{i,w}^d$  are the parameters at the same temperature and  $\tau_{w,i}^{(0)}$ ,  $\tau_{w,i}^{(1)}$ ,  $\tau_{w,i}^{(2)}$ ,  $\tau_{i,w}^{(0)}$ ,  $\tau_{i,w}^{(1)}$ , and  $\tau_{i,w}^{(2)}$  are the temperature parameters.

The final activity coefficient equation for VLE can be written as follows:

$$\ln a_w = \left( \frac{\sum_{i=1}^n (\tau_{w,i} m_i) G_{w,x}}{\sum_{i=1}^n (m_i) + m_w G_{w,x}} + \frac{\sum_{i=1}^n (\tau_{i,w} m_i) G_{x,w}}{m_w + \sum_{i=1}^n (m_i) G_{x,w}} \right) + m_w \left( \frac{-\sum_{i=1}^n (\tau_{w,i} m_i) G_{w,x}^2}{(\sum_{i=1}^n (m_i) + m_w G_{w,x})^2} - \frac{\sum_{i=1}^n (\tau_{i,w} m_i) G_{x,w}}{(m_w + \sum_{i=1}^n (m_i) G_{x,w})^2} \right) + \ln \left( \frac{(1000/Ms)}{(1000/Ms) + \sum_{i=1}^n (m_i)} \right). \quad (13)$$

In the original model, five parameters need to be correlated, and the interaction term has no physical meaning. In the new equation, two parameters ( $h$  and  $\alpha$ ) were fitted to the literature data. At the same time, the interaction parameters were given a physical meaning by the COSMO interaction. Therefore, the new model was called the NXC model.

**2.1. Calculation and Treatment of Interactions.** In this part, COSMOtherm 2021 and 1stOpt 9.0 as the main calculation tools were chosen. 1stOpt 9.0 was used to model the interaction data. COSMOtherm 2021 was chosen to calculate the intermolecular interactions in solutions. The model described above is strictly a semiempirical model. The hydration hypotheses and the model have been proposed in previous works. However, the law of microinteraction description is not clear, and the calculation result is not of physical significance. Therefore, the

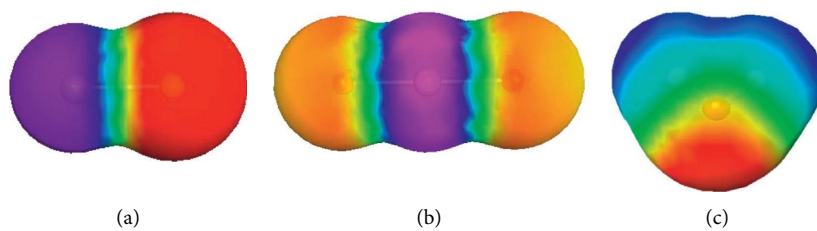
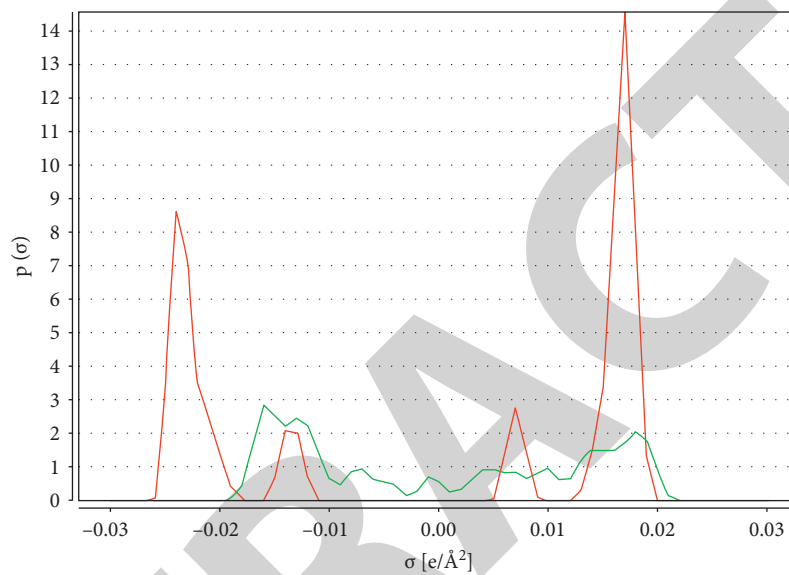
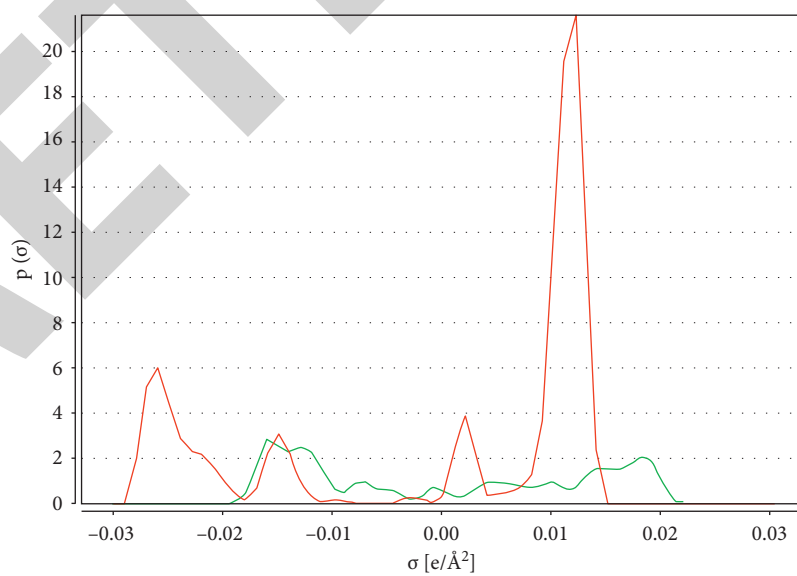
FIGURE 1: The sigma surface of NaCl, CaCl<sub>2</sub>, and H<sub>2</sub>O in COSMOtherm.FIGURE 2: The sigma profile and sigma potentials of the NaCl-H<sub>2</sub>O system (—NaCl and —H<sub>2</sub>O).FIGURE 3: The sigma profile and sigma potentials of the CaCl<sub>2</sub>-H<sub>2</sub>O system (—NaCl and —H<sub>2</sub>O).

TABLE 1: Interaction parameters 1.

	BaBr <sub>2</sub>	CaBr <sub>2</sub>	CaCl <sub>2</sub>	CsBr	CsCl
p1_1w	-1.5769E+02	-1.3593E+02	1.0610E+02	-4.0859E+02	-3.0218E+02
p1_2w	4.2414E+03	6.2605E+03	1.1310E+00	2.0634E+04	2.1218E+04
p1_3w	2.2515E+01	2.0118E+01	-1.4046E+01	5.9403E+01	4.0615E+01
p2_1w	1.8751E+01	1.2875E+02	-6.2080E-01	-1.7045E+00	7.2222E+01
p2_2w	-8.9121E+02	-6.8412E+03	-9.6625E+01	1.3260E+02	-4.0655E+03
p2_3w	-2.7893E+00	-1.8735E+01	1.2351E-01	2.4239E-01	-1.0373E+01
p3_1w	1.2176E+02	-6.6453E+01	-2.6208E+01	-2.5105E+02	-1.2997E+03
p3_2w	-2.0657E+03	2.2229E+03	-3.8316E+00	4.8514E+03	4.8162E+04
p3_3w	-2.0462E+01	9.3560E+00	-4.5660E-01	3.7830E+01	1.9558E+02
p4_1w	6.0187E+01	4.4694E+00	4.5781E-02	-7.6258E+00	6.6019E-01
p4_2w	-6.8364E+02	-2.0677E+02	-5.0076E+01	3.7699E+02	-5.7081E+01
p4_3w	-1.0406E+01	-6.7164E-01	-1.6902E-03	1.1046E+00	-9.0556E-02
p1_w1	-5.3010E+01	-8.9423E+00	-4.2979E+02	-1.8027E+02	-6.1446E+01
p1_w2	-9.4962E+01	4.9759E+02	-8.0065E+00	6.5646E+03	3.2598E+03
p1_w3	8.7205E+00	1.2512E+00	6.4195E+01	2.6804E+01	8.8857E+00
p2_w1	-4.6108E+00	-1.3330E+01	3.5584E+00	7.7152E-01	-4.2985E+01
p2_w2	-4.3741E+00	3.8167E+02	2.4795E+01	-3.1324E+01	1.1849E+03
p2_w3	7.9556E-01	1.9959E+00	-7.0131E-01	-1.1968E-01	6.7134E+00
p3_w1	1.0934E+01	-1.8255E+02	-4.7059E+02	-1.7505E+04	-2.0388E+02
p3_w2	2.0100E+02	6.6902E+03	-8.6895E+00	1.3965E+05	7.4887E+03
p3_w3	-2.3611E+00	2.7161E+01	7.7010E+01	2.9901E+03	3.0391E+01
p4_w1	8.0151E+00	1.0575E+00	-3.4347E+01	2.0544E+04	-2.2007E-02
p4_w2	-1.6102E+01	-3.2906E+01	3.3104E+01	4.3595E+01	-9.6404E-01
p4_w3	-1.3860E+00	-1.6919E-01	5.6556E+00	-3.6060E+03	2.0855E-03

TABLE 2: Interaction parameters 2.

	CsI	K <sub>2</sub> SO <sub>4</sub>	KBr	KCl	KI
p1_1w	-1.5076E+02	-1.1322E+03	-5.2890E+01	-5.4333E+02	-1.8317E+02
p1_2w	2.6520E+03	4.2812E+04	3.0350E-01	1.9740E+04	9.1426E+03
p1_3w	2.3379E+01	1.6695E+02	7.8620E+00	8.0107E+01	2.6456E+01
p2_1w	-5.8621E+00	2.6070E+00	1.1180E-01	7.6838E-01	3.4299E+00
p2_2w	2.4097E+02	-9.6319E+01	1.0920E+01	-3.7842E+01	-3.4393E+02
p2_3w	8.9043E-01	-4.0825E-01	-4.7342E-02	-1.1964E-01	-4.6963E-01
p3_1w	-2.6669E+02	1.9933E+04	-4.3606E+02	1.9205E+01	-2.6757E+02
p3_2w	1.2681E+04	-4.5828E+05	1.8225E+04	-6.4698E+02	8.5408E+03
p3_3w	3.7810E+01	-3.1560E+03	6.4023E+01	-3.0149E+00	3.9541E+01
p4_1w	7.0415E+00	1.0497E+02	-2.4939E+00	8.7763E-01	-3.7790E-02
p4_2w	-3.8769E+02	-1.1148E+05	1.0771E+02	1.1484E+03	-1.6918E+01
p4_3w	-1.0392E+00	2.6699E+01	3.7404E-01	-8.2115E-01	1.2370E-02
p1_w1	-1.8355E+02	-1.5942E+02	-1.7125E+02	-4.9179E+03	1.0020E+00
p1_w2	6.7704E+03	3.6753E+03	5.7061E+03	2.6542E+05	-4.3740E+01
p1_w3	2.7265E+01	2.6165E+01	2.5726E+01	7.1036E+02	-2.0736E-01
p2_w1	8.0511E-01	-6.8439E+00	-3.8125E-01	1.8534E+01	1.1224E+00
p2_w2	-2.6358E+01	-8.5162E+01	1.6559E+01	-3.2290E+03	5.0608E+01
p2_w3	-1.2932E-01	1.2096E+00	5.4912E-02	-3.6983E+00	-2.5325E-01
p3_w1	0.0000E+00	-3.6007E+01	-1.7478E+01	-1.8633E+02	-1.8676E+02
p3_w2	-4.8000E+01	3.7047E+03	1.3177E+03	6.8740E+03	6.9394E+03
p3_w3	2.1553E+01	2.8252E+00	2.2947E+00	2.7683E+01	2.7784E+01
p4_w1	-3.7960E+02	-3.4604E+01	-1.0760E+00	4.7385E-01	-1.9094E-01
p4_w2	3.7578E+06	1.5639E+03	6.7959E+01	-1.6643E+01	1.4145E+01
p4_w3	-3.5545E+08	5.1440E+00	1.2830E-01	-7.4893E-02	2.3459E-02

interaction term is remodeled based on COSMO calculation data. Therefore, the original model parameters were given the physical meaning of COSMO by calculation and modeling.

2.2. *The Interaction in the COSMO Calculation.* COSMOtherm 2021 (in short COSMO) is a program that computes thermophysical data for liquids. COSMO is based on the COSMO-RS theory of interacting molecular surface

TABLE 3: Interaction parameters 3.

	LiCl	MgCl <sub>2</sub>	MgSO <sub>4</sub>	Na <sub>2</sub> SO <sub>4</sub>	NaBr
p1_1w	-1.9624E+02	0.0000E+00	4.6803E+01	1.5595E+04	4.7096E+01
p1_2w	8.3829E+03	7.0357E+02	-5.9990E+04	-7.1950E+05	-2.8374E+03
p1_3w	2.9133E+01	0.0000E+00	5.0704E+01	-2.3341E+03	-7.0009E+00
p2_1w	5.6303E+00	-5.4794E+02	4.6994E+00	-1.9675E+02	-1.2808E+01
p2_2w	-3.1557E+02	-3.4876E-02	-2.7374E+02	9.3019E+03	5.0172E+02
p2_3w	-8.6033E-01	-6.2864E+01	-6.8479E-01	2.6397E+01	1.8845E+00
p3_1w	-2.4250E+02	3.1365E+00	-6.1472E+02	-7.3472E+02	-4.8166E+02
p3_2w	9.0184E+03	1.4238E+01	8.2062E+04	2.8328E+04	1.9590E+04
p3_3w	3.5512E+01	9.9977E+03	3.4574E+01	1.0841E+02	7.0887E+01
p4_1w	1.7942E+00	-1.6331E-04	5.7804E+00	2.0889E+00	-1.3560E+00
p4_2w	-8.3372E+01	-5.5570E+01	-3.3880E+02	-8.3239E+01	5.7880E+01
p4_3w	-2.7306E-01	-1.5810E+02	-8.4090E-01	-3.2257E-01	1.9850E-01
p1_w1	-1.6909E+02	-3.4915E+01	-1.8918E+02	-1.9473E+02	-1.2532E+02
p1_w2	6.1039E+03	-8.0377E+01	7.0911E+03	8.2187E+03	4.0464E+03
p1_w3	2.5139E+01	-1.5844E+01	2.8073E+01	2.8559E+01	1.8727E+01
p2_w1	8.4758E-01	-2.3443E+00	2.8420E+00	-1.9109E+00	1.3881E+00
p2_w2	-3.6891E+01	1.2393E+02	-1.1058E+02	1.1746E+02	-6.3787E+01
p2_w3	-1.2922E-01	2.8080E-01	-4.4140E-01	2.6448E-01	-2.0735E-01
p3_w1	-2.2090E+01	2.4764E+01	-7.5304E+01	4.2513E+00	-5.8272E+01
p3_w2	1.1497E+03	4.2759E+01	-6.1590E+00	-1.0872E+03	2.7566E+03
p3_w3	3.1878E+00	1.5251E+01	-2.2653E+01	-2.9049E-01	8.5269E+00
p4_w1	-1.8311E+01	3.1783E+01	2.5633E+01	-9.4684E-01	9.1862E-01
p4_w2	1.5655E+03	-1.8591E+02	-2.0188E+03	-4.3411E+01	1.6165E+01
p4_w3	2.2754E+00	-5.4919E+00	-6.6956E+00	1.9837E-01	-1.9654E-01

TABLE 4: Interaction parameters 4.

	NaCl	NaI	RbCl	SrCl <sub>2</sub>	ZnCl <sub>2</sub>
p1_1w	-1.1661E+02	-4.0262E+02	-1.4861E+02	-1.4894E+02	6.6039E+03
p1_2w	4.9274E+01	1.7533E+04	7.9653E+03	2.9476E+03	-2.0810E+05
p1_3w	1.7656E+01	5.8586E+01	2.1317E+01	2.2622E+01	-5.4124E+02
p2_1w	2.0329E+00	-7.0058E-01	-2.0617E+00	4.9975E+00	-3.4050E+02
p2_2w	-1.0981E+02	3.4959E+01	5.5783E+01	-2.5181E+02	5.8513E+03
p2_3w	-2.9922E-01	9.5589E-02	3.4073E-01	-7.3430E-01	3.6359E+01
p3_1w	-3.1042E+02	3.0597E+01	-6.0264E+02	-1.7136E+02	-7.3847E+01
p3_2w	1.5486E+04	-2.5349E+03	2.1380E+04	8.2118E+03	2.9548E+03
p3_3w	4.5170E+01	-4.1664E+00	8.9281E+01	2.4363E+01	1.0794E+01
p4_1w	1.2298E+02	-3.3004E+01	-6.8398E-01	1.6381E+01	4.6732E+00
p4_2w	-6.0785E+03	1.5906E+03	5.3327E+01	-9.4137E+02	-2.2010E+02
p4_3w	-1.8096E+01	4.7729E+00	8.1138E-02	-2.3786E+00	-7.0826E-01
p1_w1	-1.3776E+02	6.4223E+01	-5.8723E+01	2.6023E+00	-7.8527E+01
p1_w2	4.4852E+03	-3.9484E+03	3.2642E+03	9.2837E+00	3.0765E+03
p1_w3	2.0579E+01	-9.3726E+00	8.4339E+00	-4.7917E-01	1.1595E+01
p2_w1	1.8386E+00	1.8314E-01	5.6485E-01	-8.3981E+00	6.3595E+00
p2_w2	-8.8162E+01	-1.5504E-03	-2.6417E+01	-3.6593E+00	-1.8121E+02
p2_w3	-2.7270E-01	-4.4962E-02	-6.2320E-02	1.3420E+00	-1.0067E+00
p3_w1	-9.6971E+01	-2.5433E+02	-1.2644E+02	-1.9611E+02	-9.3813E+01
p3_w2	4.7896E+03	1.1051E+04	3.5827E+03	7.2753E+03	3.1889E+03
p3_w3	1.4194E+01	3.7594E+01	1.9064E+01	2.9190E+01	1.4000E+01
p4_w1	-2.7864E+01	-3.8597E+00	-3.4679E-01	-2.2429E-01	2.9848E+00
p4_w2	1.1229E+03	1.9773E+02	3.6769E+01	1.8740E+01	-1.9860E+02
p4_w3	4.1234E+00	5.6372E-01	3.9342E-02	2.4635E-02	-4.1453E-01

charges [29, 30]. For the calculation of intermolecular interactions, the COSMO-chemical potential-mixture module was used. Before the calculation, compound details need to

be entered. There are two main ways to input the components: one is to select the compounds directly in the database, and the other is to establish the new compounds in

TABLE 5: Correlation of VLE data.

System	T/K	Data points	This work		Reference and experiment
			dY/kPa <sup>a</sup>	dP/% <sup>b</sup>	
BaBr <sub>2</sub>	298.15 to 343.15	63	0.058	0.81	[31, 32]
CaBr <sub>2</sub>	298.15 to 343.15	63	0.053	1.13	[31, 32]
CaCl <sub>2</sub>	273.15 to 415.15	236	0.457	1.19	[9, 16, 31, 32]
CsBr	298.15 to 343.15	51	0.064	0.71	[31, 32]
CsCl	298.15 to 343.15	63	0.457	1.19	[31, 32]
CsI	298.15 to 343.15	42	0.032	0.54	[31, 32]
K <sub>2</sub> SO <sub>4</sub>	298.15 to 373.65	104	1.067	2.72	[9, 32]
KBr	298.15 to 343.15	51	0.251	3.28	[31, 32]
KCl	273.15 to 343.15	66	0.194	2.50	[9, 16, 31, 32]
KI	298.15 to 343.15	60	0.188	2.24	[31, 32]
LiCl	298.15 to 394.4	47	0.011	0.42	[32, 33]
MgCl <sub>2</sub>	298.15 to 377.85	120	0.490	1.86	[9, 31, 32]
MgSO <sub>4</sub>	273.15 to 376.45	120	0.810	1.85	[9, 31, 32]
Na <sub>2</sub> SO <sub>4</sub>	273.15 to 298.15	30	0.009	0.46	[9, 32]
NaBr	298.15 to 343.15	47	0.011	0.21	[31, 32]
NaCl	298.15 to 373.15	89	0.097	0.92	[31, 32]
NaI	298.15 to 343.15	58	0.420	3.92	[31, 32]
RbCl	298.15 to 343.15	51	0.293	3.12	[31, 32]
SrCl <sub>2</sub>	298.15 to 343.15	59	0.230	3.13	[31, 32]
ZnCl <sub>2</sub>	298.15 to 379.8	23	0.008	0.031	[32, 33]
Average			0.26	1.611	

<sup>a</sup>dY = (1/N) ∑ |P<sub>exp</sub> - P<sub>cal</sub>|, where N is the number of data points. <sup>b</sup>dP = (1/N) ∑ |P<sub>exp</sub> - P<sub>cal</sub>|/P<sub>exp</sub> × 100%, where N is the number of data points. P<sub>exp</sub> represents the experimental pressure and P<sub>cal</sub> represents the calculated pressure.

TABLE 6: The parameters  $\alpha$  and  $h_i$ .

	BaBr <sub>2</sub>	CaBr <sub>2</sub>	CaCl <sub>2</sub>	CsBr	CsCl
A	7.9752E - 02	2.8767E - 01	1.6389E - 01	6.7821E - 15	4.5910E - 01
$h_i$	4.6147E + 00	5.6968E + 00	2.3336E + 00	-8.4186E - 01	-3.8792E - 01
	CsI	K <sub>2</sub> SO <sub>4</sub>	KBr	KCl	KI
A	1.1545E - 14	5.9029E - 01	2.6438E - 02	9.8801E - 03	2.4789E - 02
$h_i$	-4.6851E - 01	-1.7788E + 01	-5.0900E + 00	-4.9304E + 00	-2.5134E + 00
	LiCl	MgCl <sub>2</sub>	MgSO <sub>4</sub>	Na <sub>2</sub> SO <sub>4</sub>	NaBr
A	8.1229E - 02	2.4432E - 03	3.2566E - 01	4.4404E - 01	3.4094E - 02
$h_i$	1.6472E + 00	6.2690E + 00	9.8217E + 00	-2.4529E + 00	1.4730E - 01
	NaCl	NaI	RbCl	SrCl <sub>2</sub>	ZnCl <sub>2</sub>
A	-5.8248E - 01	-4.9761E - 01	-1.3570E - 03	8.2369E - 02	7.1066E - 01
$h_i$	3.6925E + 00	5.3929E + 00	-2.4792E + 00	3.5726E + 00	6.2096E + 00

COSMO-TmoleX. Because the ion pairs and hydration assumptions are involved in the new model, COSMO-TmoleX is selected.

The calculation process is as follows:

- (1) The necessary step needs to create a new ion pair "molecular" in TmoleX and optimize the structural formula, such as the sigma surface of NaCl, CaCl<sub>2</sub>, and H<sub>2</sub>O shown in Figure 1.
- (2) According to the optimization results, a preliminary study on the new ion pair "molecular" is conducted. Sigma profile/potentials are important interaction reference indicators, such as Figures 2 and 3.
- (3) The next step is as follows: open chemical potential-mixture in COSMOtherm 2021.

- (4) When determining the compound, it is necessary to input the temperature and liquid phase composition and add a calculation table.

- (5) Run the job to get the data.

2.3. *The Results of COSMO Calculation.* When the calculation is completed, the calculation results are analyzed. From the COSMO calculation results, it can be seen that some related data can be obtained, such as the chemical potential of the compound in the mixture, the total mean interaction energy in the mix (H<sub>int</sub>), the misfit interaction energy in the mix (H<sub>MF</sub>), the H-bond interaction energy in the mix (H<sub>HB</sub>), and the vdW interaction energy in the mix (H<sub>vdW</sub>).

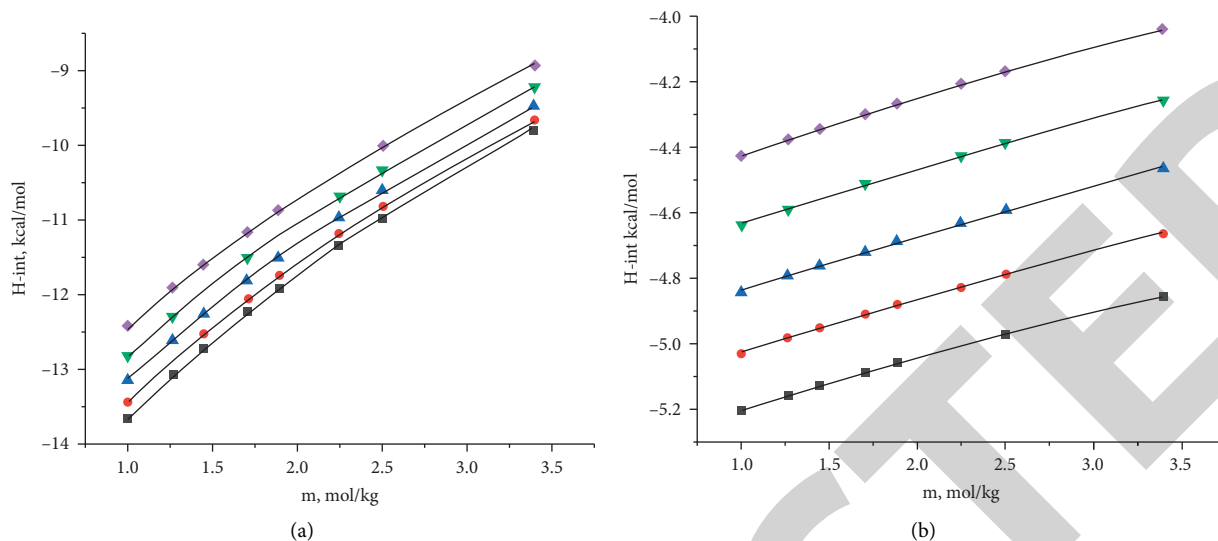


FIGURE 4: Correlation of the interaction data for the BaBr<sub>2</sub>+H<sub>2</sub>O system. (a) The interaction of BaBr<sub>2</sub> and (b) the interaction of H<sub>2</sub>O. Symbols (■, T = 303.15 K; ●, T = 313.15 K; ▲, T = 323.15 K; ▼, T = 333.15 K; and ◆, T = 343.15 K); COSMO data; lines: correlation.

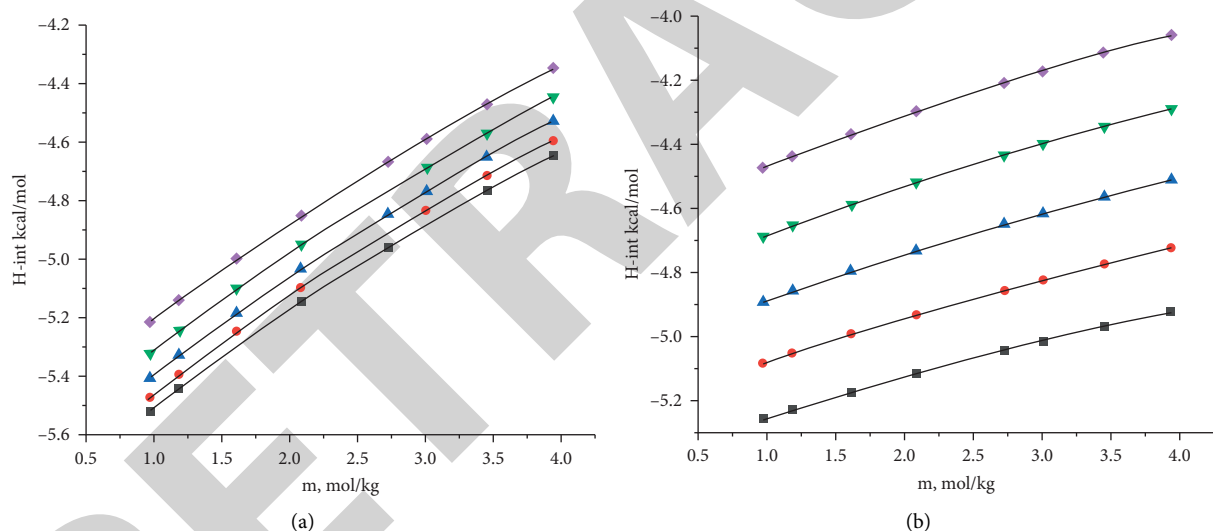


FIGURE 5: Correlation of the interaction data for the CaBr<sub>2</sub>+H<sub>2</sub>O system. (a) The interaction of CaBr<sub>2</sub> and (b) the interaction of H<sub>2</sub>O. Symbols (■, T = 303.15 K; ●, T = 313.15 K; ▲, T = 323.15 K; ▼, T = 333.15 K; and ◆, T = 343.15 K); COSMO data; lines: correlation.

In the model section, equations (5) ~ (8) are the main interaction terms. They described the total interaction. So, the total mean interaction energy ( $H_{int}$ ) in COSMOtherm is used as the main research object.

**2.4. Modeling of the  $H_{int}$  Interaction by 1stOpt.** When the  $H_{int}$  interaction calculation was completed, we modeled the data and established the equations. Then, the established equations were added to the NXC model. During the modeling process, Quick Fit in 1stopt 9.0 was used to model the  $H_{int}$  interaction equations. For this fitting, out of 100,000 equations, the best model was searched. The optimal equation forms are given as follows:

$$\tau_x = \sum_{i=1}^n (\tau_i^a \exp(\tau_i^b m_i) + \tau_i^c \exp(\tau_i^d m_i)), \quad (14)$$

$$\tau_i^x = \frac{\tau_i^{(0)} + \tau_i^{(1)}}{T + \tau_i^{(2)} \ln(T)}. \quad (15)$$

After the formulas were determined, the next important step was to fit the parameters for the above equations. These parameters are of physical significance in COSMO, and the interaction terms in the model also have a physical meaning. The parameter fitting was also performed by using 1stopt 9.0. The interaction parameters are listed in Tables 1~4.



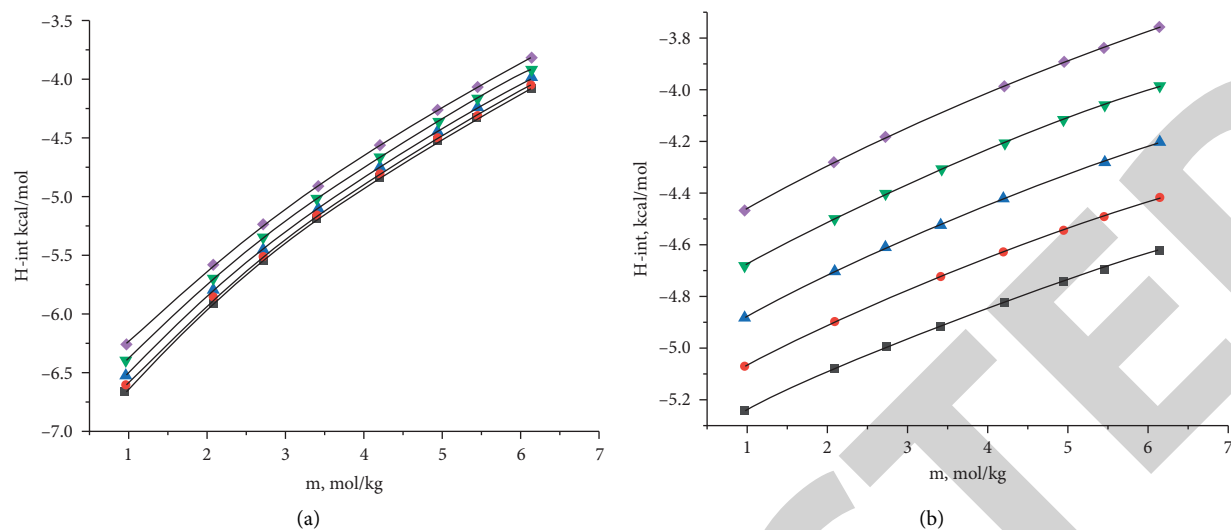


FIGURE 6: Correlation of the interaction data for the CaCl<sub>2</sub>+H<sub>2</sub>O system. (a) The interaction of CaCl<sub>2</sub> and (b) the interaction of H<sub>2</sub>O. Symbols (■, T = 303.15 K; ●, T = 313.15 K; ▲, T = 323.15 K; ▼, T = 333.15 K; and ◆, T = 343.15 K); COSMO data; lines: correlation.

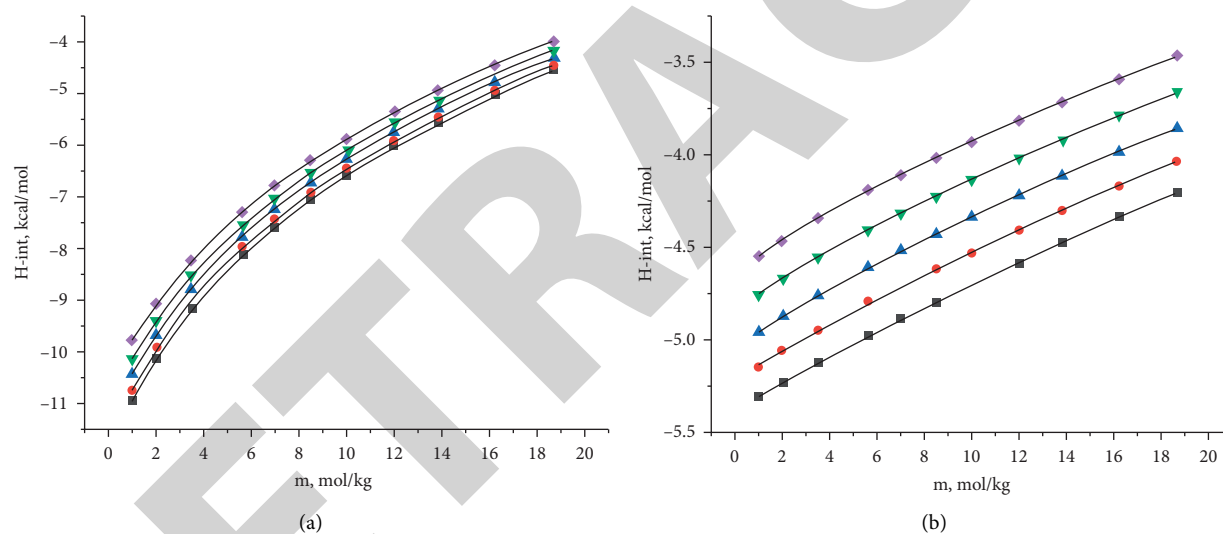


FIGURE 7: Correlation of the interaction data for the LiCl + H<sub>2</sub>O system. (a) The interaction of LiCl and (b) the interaction of H<sub>2</sub>O. Symbols (■, T = 303.15 K; ●, T = 313.15 K; ▲, T = 323.15 K; ▼, T = 333.15 K, and ◆, T = 343.15 K); COSMO data; lines: correlation.

TABLE 7: Correlation of H int data.

System	T/K	Salt-water interaction		Water-salt interaction	
		dY/kcal.mol <sup>-1a</sup>	dP/% <sup>b</sup>	dY/kcal.mol <sup>-1a</sup>	dP/% <sup>b</sup>
BaBr <sub>2</sub>	298.15 to 343.15	0.0105	0.0944	0.0024	0.0504
CaBr <sub>2</sub>	298.15 to 343.15	0.0001	0.0183	0.0003	0.0077
CaCl <sub>2</sub>	298.15 to 343.15	0.0013	0.0258	0.0004	0.0092
CsBr	298.15 to 343.15	0.0044	0.0261	0.0018	0.0385
CsCl	298.15 to 343.15	0.0144	0.0796	0.0015	0.0319
CsI	298.15 to 343.15	0.0005	0.0037	0.0007	0.6001
K <sub>2</sub> SO <sub>4</sub>	298.15 to 343.15	0.0072	0.0216	0.0009	0.0186
KBr	298.15 to 343.15	0.0031	0.0217	0.0015	0.0321
KCl	298.15 to 343.15	0.0073	0.0427	0.0021	0.0425
KI	298.15 to 343.15	0.0053	0.0423	0.0007	0.0172
LiCl	298.15 to 343.15	0.0067	0.1118	0.0029	0.0682
MgCl <sub>2</sub>	298.15 to 343.15	0.0254	0.8672	0.0029	0.0693

TABLE 7: Continued.

System	T/K	Salt-water interaction		Water-salt interaction	
		dY/kcal.mol <sup>-1a</sup>	dP/% <sup>b</sup>	dY/kcal.mol <sup>-1a</sup>	dP/% <sup>b</sup>
MgSO <sub>4</sub>	298.15 to 343.15	0.0408	2.7068	0.0021	0.0517
Na <sub>2</sub> SO <sub>4</sub>	298.15 to 343.15	0.0124	0.0688	0.0009	0.0187
NaBr	298.15 to 343.15	0.0034	0.0319	0.0024	0.0531
NaCl	298.15 to 343.15	0.0081	0.0614	0.0015	0.0335
NaI	298.15 to 343.15	0.0032	0.0369	0.0031	0.0699
RbCl	298.15 to 343.15	0.0183	0.0995	0.0031	0.0645
SrCl <sub>2</sub>	298.15 to 343.15	0.0176	0.1568	0.0007	0.0147
ZnCl <sub>2</sub>	298.15 to 343.15	0.0098	0.6254	0.0037	0.0812
Average		0.010	0.257	0.0018	0.0689

<sup>a</sup>dY = (1/N) ∑ |P<sub>exp</sub> - P<sub>cal</sub>|, where N is the number of data points. <sup>b</sup>dP = (1/N) ∑ |P<sub>exp</sub> - P<sub>cal</sub>|/P<sub>exp</sub> × 100%, where N is the number of data points. P<sub>exp</sub> represents the experimental pressure and P<sub>cal</sub> represents the calculated pressure.

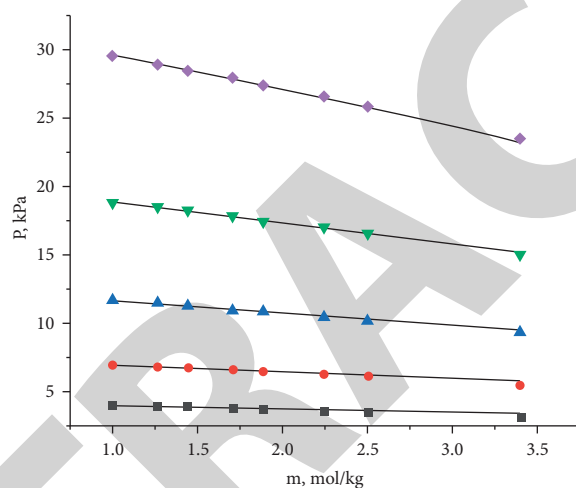


FIGURE 8: Calculation of the VLE for the BaBr<sub>2</sub>+H<sub>2</sub>O system. Symbols (■, T = 303.15 K; ●, T = 313.15 K; ▲, T = 323.15 K; ▼, T = 333.15 K; and ◆, T = 343.15 K); VLE data; lines: calculation.

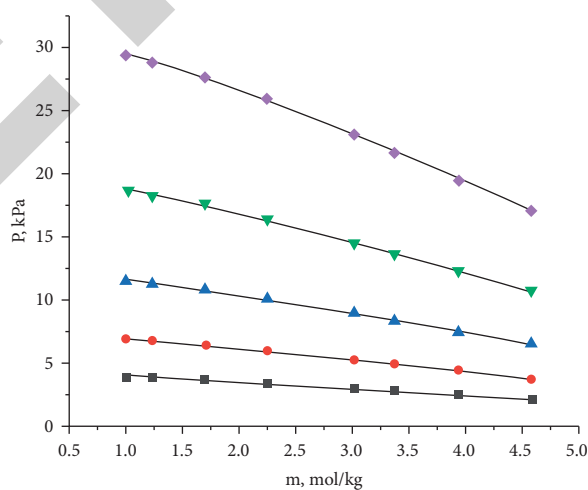


FIGURE 9: Calculation of the VLE for the CaBr<sub>2</sub>+H<sub>2</sub>O system. Symbols (■, T = 303.15 K; ●, T = 313.15 K; ▲, T = 323.15 K; ▼, T = 333.15 K; and ◆, T = 343.15 K); VLE data; lines: calculation.

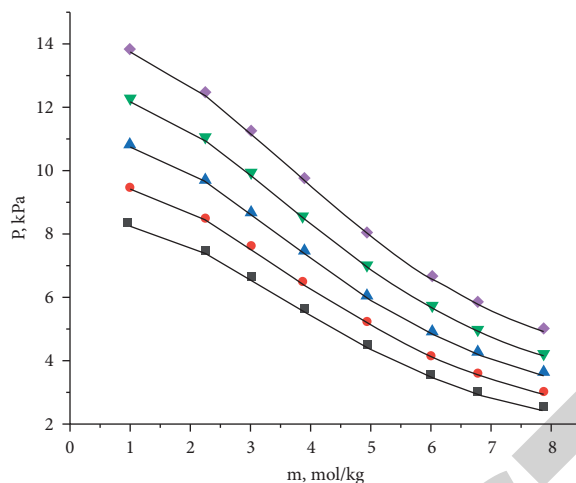


FIGURE 10: Calculation of the VLE for the CaCl<sub>2</sub>+H<sub>2</sub>O system. Symbols (■, T = 303.15 K; ●, T = 313.15 K; ▲, T = 323.15 K; ▼, T = 333.15 K; and ◆, T = 343.15 K); VLE data; lines: calculation.

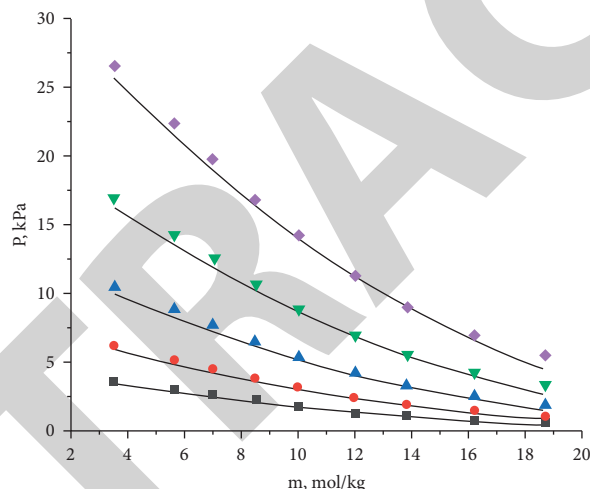


FIGURE 11: Calculation of the interaction data for the LiCl + H<sub>2</sub>O system. Symbols (■, T = 303.15 K; ●, T = 313.15 K; ▲, T = 323.15 K; ▼, T = 333.15 K, and ◆, T = 343.15 K); VLE data; lines: calculation.

Through the above derivation and processing, final model equations (9) ~ (14) were determined. Parameters  $\tau_{w,i}^{(x-0)}$ ,  $\tau_{w,i}^{(x-1)}$ ,  $\tau_{w,i}^{(x-2)}$ ,  $\tau_{i,w}^{(x-0)}$ ,  $\tau_{i,w}^{(x-1)}$ , and  $\tau_{i,w}^{(x-2)}$  were fitted on the basis of the COSMO data. Therefore, it only needs to fit the parameters  $\alpha$  and  $h_i$  on the basis of the VLE data.

**2.5. Determination of the Parameters  $\alpha$  and  $h_i$ .** The determination of the model parameters is a critical step in this paper. The interaction parameters were determined based on the COSMO data. Parameters  $\alpha$  and  $h_i$  are further correlated by using phase equilibrium data. The data used for correlation are VLE data, and the references are listed in Table 5. The parameters  $\alpha$  and  $h_i$  are listed in Table 6.

### 3. Results and Discussion

**3.1. The Results of Interaction and Parameters.** In data processing, it can be found that H<sub>int</sub> energy is related to concentration, temperature, etc. From Figures 4~7, it can be

seen that the energy increases with temperature and concentration.

Equations (13) and (14) were used to correlate the H<sub>int</sub> interaction. The calculation results are listed in Table 7. For all systems in this paper, the results show that  $dY \leq 0.0408$  kcal/mol and the average of  $dY = 0.0058$  kcal/mol and  $dP \leq 2.71\%$  and the average of  $dP = 0.162\%$ . So, the equations can be better used to describe the change of H<sub>int</sub> energy.

$$dY = \left(\frac{1}{N}\right) \sum |P_{\text{exp}} - P_{\text{cal}}|, \quad (16)$$

$$dP = \frac{(1/N) \sum |P_{\text{exp}} - P_{\text{cal}}|}{P_{\text{exp}} \times 100\%}. \quad (17)$$

**3.2. Prediction of the VLE Data in Electrolyte Solutions.** The modified model and parameters described above were used to calculate the VLE data for twenty electrolyte

TABLE 8: Calculations for VLE data.

System	T/Kact	This work		Previous work	
		dY/kPa <sup>a</sup>	dP/% <sup>b</sup>	dY/kPa <sup>a</sup>	dP/% <sup>b</sup>
BaBr <sub>2</sub>	298.15 to 343.15	0.058	0.81	0.079	0.78
CaBr <sub>2</sub>	298.15 to 343.15	0.053	1.13	0.049	1.1
CaCl <sub>2</sub>	273.15 to 415.15	0.457	1.19	0.081	1.82
CsBr	298.15 to 343.15	0.064	0.71	0.097	1.01
CsCl	298.15 to 343.15	0.457	1.19	0.091	0.97
CsI	298.15 to 343.15	0.032	0.54	0.039	0.42
K <sub>2</sub> SO <sub>4</sub>	298.15 to 373.65	1.067	2.72	0.051	1.15
KBr	298.15 to 343.15	0.251	3.28	0.077	0.87
KCl	273.15 to 343.15	0.194	2.50	0.044	0.67
KI	298.15 to 343.15	0.188	2.24	0.097	0.95
LiCl	298.15 to 394.4	0.011	0.42	0.018	1.25
MgCl <sub>2</sub>	298.15 to 377.85	0.490	1.86	0.07	1
MgSO <sub>4</sub>	273.15 to 376.45	0.810	1.85	0.076	0.85
Na <sub>2</sub> SO <sub>4</sub>	273.15 to 298.15	0.009	0.46	0.012	0.53
NaBr	298.15 to 343.15	0.011	0.21	0.048	0.75
NaCl	298.15 to 373.15	0.097	0.92	0.04	0.65
NaI	298.15 to 343.15	0.420	3.92	0.09	0.929
RbCl	298.15 to 343.15	0.293	3.12	0.061	0.69
SrCl <sub>2</sub>	298.15 to 343.15	0.230	3.13	0.068	0.71
ZnCl <sub>2</sub>	298.15 to 379.8	0.008	0.031	0.03	1
Average		0.26	1.61	0.061	0.905

<sup>a</sup>dY = (1/N) ∑ |P<sub>exp</sub> - P<sub>cal</sub>|, where N is the number of data points. <sup>b</sup>dP = (1/N) ∑ |P<sub>exp</sub> - P<sub>cal</sub>|/P<sub>exp</sub> × 100%, where N is the number of data points.

solutions at vapor pressures ranging between 6 kPa and 101.325 kPa. The results of the calculation are presented in Table 5, and dY and dP are listed in Table 8.

For all systems in this paper, the results show that dY ≤ 1.067 kPa and the average of dY = 0.26 kPa and dP ≤ 3.92% and the average of dP = 3.92%. The calculation results for the VLE data are shown in Figure 8–11 for BaBr<sub>2</sub>, CaBr<sub>2</sub>, CaCl<sub>2</sub>, and LiCl systems, respectively.

**3.3. Comparison with the Results Obtained from the Previous Model.** Some systems were selected to compare the results obtained in this paper and previous calculations. The results of the comparisons are shown in Table 8. From the results, it can be concluded that the maximum dY of the developed model is 1.067 kPa and that the maximum dP is 3.92%. Similarly, the average dY is 0.26 kPa, and the average dP is 1.61%. In general, the results of the model calculations in this paper are not as good as those reported previously, but the parameters are given better physical meaning, and the number of parameters used is lower.

## 4. Conclusions

Modeling and calculation of VLE for an electrolyte solution are studied in this paper. Based on previous works, a developed NRTL model is proposed. The influence mechanism for the microscopic interaction on macroscopic VLE is further studied by COSMOtherm. It can be obtained from the calculation result of COSMOtherm that the temperature and concentration of electrolyte solutions are higher, and the interaction energy (H<sub>int</sub>) is larger. The interaction parameters in the model are

successfully linked to the COSMO interaction energy (H<sub>int</sub>) and given a new physical meaning. The model can be used to successfully predict the VLE data for electrolyte solutions at vapor pressures ranging between 6 kPa and 101.325 kPa. It is suitable for most electrolyte solutions. Although the calculation results are slightly inferior to those of previous works, there is an important significance for the establishment of the model framework in this work.

## Data Availability

The data used to support the findings of this study are included within the article.

## Conflicts of Interest

The authors declare that they have no conflicts of interest.

## Acknowledgments

This work was supported by the National Natural Science Foundation of China (Grant 273 nos. 22073054 and 21703115).

## References

- [1] M. Costa Reis, "Ion activity models: the Debye-Hückel equation and its extensions," *ChemTexts*, vol. 7, no. 2, p. 9, 2021.
- [2] J. M. Prausnitz, R. N. Lichtenthaler, and E. Azevedo, "Molecular thermodynamics of fluid-phase equilibria," *Thermodynamics*, 1999.

- [3] K. S. Pitzer, "Thermodynamics of electrolytes. I. Theoretical basis and general equations," *Journal of Physical Chemistry*, vol. 77, no. 2, pp. 268–277, 1973.
- [4] A. C. Galvão, Y. P. Jiménez, F. J. Justel, W. S. Robazza, and F. S. Donatti, "Salting-out precipitation of NaCl, KCl and NH<sub>4</sub>Cl in mixtures of water and methanol described by the modified Pitzer model," *The Journal of Chemical Thermodynamics*, vol. 150, Article ID 106202, 2020.
- [5] J. D. Toner, D. C. Catling, and B. Light, "A revised Pitzer model for low-temperature soluble salt assemblages at the Phoenix site, Mars," *Geochimica et Cosmochimica Acta*, vol. 166, pp. 327–343, 2015.
- [6] R. H. Stokes and R. A. Robinson, "Solvation equilibria in very concentrated electrolyte solutions," *Journal of Solution Chemistry*, vol. 2, no. 2-3, pp. 173–191, 1973.
- [7] X. H. Lu and G. Maurer, "Model for describing activity coefficients in mixed electrolyte aqueous solutions," *AIChE Journal*, vol. 39, no. 9, pp. 1527–1538, 1993.
- [8] G. M. Wilson, "Vapor-liquid equilibrium XI. A new expression for the excess free energy of mixing," *Journal of the American Chemical Society*, vol. 86, no. 2, pp. 127–130, 1964.
- [9] H. Renon and J. M. Prausnitz, "Local compositions in thermodynamic excess functions for liquid mixtures," *AIChE Journal*, vol. 14, no. 1, pp. 135–144, 1968.
- [10] D. S. Abrams and J. M. Prausnitz, "Statistical thermodynamics of liquid mixtures: a new expression for the excess Gibbs energy of partly or completely miscible systems," *AIChE Journal*, vol. 21, no. 1, pp. 116–128, 1975.
- [11] C. C. Chen, H. I. Britt, J. F. Boston, and L. B. Evans, "Local composition model for excess Gibbs energy of electrolyte systems. Part I: single solvent, single completely dissociated electrolyte systems," *AIChE Journal*, vol. 28, no. 4, pp. 588–596, 1982.
- [12] C. C. Chen and L. B. Evans, "A local composition model for the excess Gibbs energy of aqueous electrolyte systems," *AIChE Journal*, vol. 32, no. 3, pp. 444–454, 1986.
- [13] P. Wang, A. Anderko, and R. D. Young, "A speciation-based model for mixed-solvent electrolyte systems," *Fluid Phase Equilibria*, vol. 203, no. 1-2, pp. 141–176, 2002.
- [14] K. Thomsen and P. Rasmussen, "Modeling of vapor-liquid-solid equilibrium in gas-aqueous electrolyte systems," *Chemical Engineering Science*, vol. 54, no. 12, pp. 1787–1802, 1999.
- [15] J. Gmehling, J. D. Li, and M. Schiller, "A modified unifac model .2. Present parameter matrix and results for different thermodynamic properties," *Industrial & Engineering Chemistry Research*, vol. 32, no. 1, pp. 178–193, 1993.
- [16] X. Xu, Y. Hu, X. Wang, and L. Wu, "Experimental and modeling of vapor-liquid equilibria for mixed electrolyte solution systems," *Journal of Chemical & Engineering Data*, vol. 61, no. 7, pp. 2311–2320, 2016.
- [17] D. Li, D. Zeng, H. Han, L. Guo, X. Yin, and Y. Yao, "Phase diagrams and thermochemical modeling of salt lake brine systems. I. LiCl+H<sub>2</sub>O system," *Calphad*, vol. 51, pp. 1–12, 2015.
- [18] J. Gross and G. Sadowski, "Application of perturbation theory to a hard-chain reference fluid: an equation of state for square-well chains," *Fluid Phase Equilibria*, vol. 168, no. 2, pp. 183–199, 2000.
- [19] Y. Iwai and K. Matsubara, "Simultaneous correlation of liquid-liquid equilibria for ternary systems and phase equilibria for constituent binary systems by modified new activity coefficient model," *Fluid Phase Equilibria*, vol. 556, Article ID 113411, 2022.
- [20] A. Noumir and B. Saad, "Modeling of isobaric vapor-liquid equilibrium data for ionic liquid-containing ternary systems," *Russian Journal of Physical Chemistry*, vol. 96, no. 1, pp. 27–35, 2022.
- [21] S. Chen, M. Wang, J. Hu, Y. Guo, and T. Deng, "Phase equilibria in the aqueous ternary systems (NaCl + NaBO<sub>2</sub> + H<sub>2</sub>O) and (Na<sub>2</sub>SO<sub>4</sub> + NaBO<sub>2</sub> + H<sub>2</sub>O) at 298.15 K and 0.1 MPa," *Journal of Chemical & Engineering Data*, vol. 63, no. 12, pp. 4662–4668, 2018.
- [22] L. Meng, M. S. Gruszkiewicz, T. Deng, Y. Guo, and D. Li, "Isoopiestic measurements of thermodynamic properties for the aqueous system LiBr–CaBr<sub>2</sub>–H<sub>2</sub>O at 373.15 K," *The Journal of Chemical Thermodynamics*, vol. 129, pp. 83–91, 2019.
- [23] J. Zhou, Y. Zeng, G. P. Demopoulos, C. Li, and Z. Li, "Solubility of NaHCO<sub>3</sub> and NH<sub>4</sub>HCO<sub>3</sub> in the relevant media and prediction of high-pressure phase equilibria for the NH<sub>3</sub>–CO<sub>2</sub>–NaCl–H<sub>2</sub>O system," *Journal of Chemical & Engineering Data*, vol. 62, no. 12, pp. 4401–4410, 2017.
- [24] C. K. Chang, W. L. Chen, D. T. Wu, and S. T. Lin, "Improved directional hydrogen bonding interactions for the prediction of activity coefficients with COSMO-SAC," *Industrial & Engineering Chemistry Research*, vol. 57, no. 32, pp. 11229–11238, 2018.
- [25] T. Gerlach, T. Ingram, G. Sieder, and I. Smirnova, "Modeling the solubility of CO<sub>2</sub> in aqueous methyl diethanolamine solutions with an electrolyte model based on COSMO-RS," *Fluid Phase Equilibria*, vol. 461, pp. 39–50, 2018.
- [26] M. Królikowska, M. Skonieczny, K. Padaszyński, and M. Zawadzki, "Vapor pressure and physicochemical properties of {LiBr + IL-based additive + water} mixtures: experimental data and COSMO-RS predictions," *Journal of Solution Chemistry*, vol. 50, no. 4, pp. 473–502, 2021.
- [27] X. Xu, Y. Zhou, Z. Wang, and X. Wang, "Experiment and modeling of vapor-liquid equilibria for H<sub>2</sub>O+CH<sub>3</sub>OH+KCl and H<sub>2</sub>O+CH<sub>3</sub>OH+NaBr systems," *Calphad*, vol. 63, pp. 134–141, 2018.
- [28] X. Xu, N. Zhang, Y. Zhou, Y. Wang, and Z. Wang, "The effects of NaI, KBr, and KI salts on the vapor-liquid equilibrium of the H<sub>2</sub>O+CH<sub>3</sub>OH system," *Frontiers of Chemistry*, vol. 8, 2020.
- [29] F. Eckert and A. Klamt, "Fast solvent screening via quantum chemistry: COSMO-RS approach," *AIChE Journal*, vol. 48, no. 2, pp. 369–385, 2002.
- [30] A. Klamt and F. Eckert, "COSMO-RS: a novel and efficient method for the a priori prediction of thermophysical data of liquids," *Fluid Phase Equilibria*, vol. 172, no. 1, pp. 43–72, 2000.
- [31] K. R. Patil, A. D. Tripathi, G. Pathak, and S. S. Katti, "Thermodynamic properties of aqueous electrolyte solutions. 2. Vapor pressure of aqueous solutions of sodium bromide, sodium iodide, potassium chloride, potassium bromide, potassium iodide, rubidium chloride, cesium chloride, cesium bromide, cesium iodide, magnesium chloride, calcium chloride, calcium bromide, calcium iodide, strontium chloride, strontium bromide, strontium iodide, barium chloride,

- and barium bromide," *Journal of Chemical & Engineering Data*, vol. 36, pp. 225–230, 1991.
- [32] R. A. Robinson and R. H. Stokes, *Electrolyte Solutions*, Courier Corporation, Chelmsford, MA, USA, 2002.
- [33] P. Kolář, H. Nakata, A. Tsuboi, P. Wang, and A. Anderko, "Measurement and modeling of vapor–liquid equilibria at high salt concentrations," *Fluid Phase Equilibria*, vol. 228–229, pp. 493–497, 2005.
- [34] R. F. Platford, "Osmotic coefficients of aqueous solutions of seven compounds at 0.deg," *Journal of Chemical & Engineering Data*, vol. 18, no. 2, pp. 215–217, 1973.

RETRACTED