Solubility of dilute SO$_2$ in DMSO Mn^2 mixture solvents and EOS model-(II)

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On the basis of solubility measurement of dilute SO_2 in $DMSO + Mn^{2+}$ mixture solvents, a new EOS model was established to represent gas–liquid equilibrium system, and the solubilities calculated by the model show good agreement with experimental data.

Keywords: Solubility; Gas–liquid equilibrium; Sulfur dioxide; EOS

1. Introduction

On the basis of solubility measurement of dilute SO_2 in $DMSO + Mn^{2+}$ mixture solvents, we established an EOS model based on experimental data. This model is set out in detail in section 2 immediately below. A summary is presented in section 3.

2. The EOS model

In the literature, the various models used to obtain a representation of gas in electrolyte solution systems may be divided into three kinds of approaches: The first one corresponds to empirical treatments. However, its extrapolation capabilities are weak. The second approach is based on an excess Gibbs energy model. In the last kind of approach, equations of state are used. The EOS approach is better than other approaches, because the same reference states were adopted for liquid and gas phases, on Henry constants being needed in this case. Furthermore, the EOS approach is more simple and practical than the excess Gibbs energy model, for some systems that haven't the excess Gibbs energy expression, it can be represented by the EOS.

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Therefore in this study, on the basis of the EOS derived by Furst [1], a new EOS model has been established to represent gas–liquid equilibrium.

2.1. *The expression of Helmholtz energy for electrolyte solution*

In this model the molar of Helmholtz energy is developed as the sum of four contributions, considering interaction energy between ions and solvent and between cations and anions on the basis of EOS derived by Furst *et al.* [1–7]

$$\left(\frac{\Delta A}{RT}\right) = \left(\frac{\Delta A}{RT}\right)_{RF} + \left(\frac{\Delta A}{RT}\right)_{SR1} + \left(\frac{\Delta A}{RT}\right)_{SR2} + \left(\frac{\Delta A}{RT}\right)_{LR}. \tag{1}$$

The first term (RF) is relative to repulsive forces, the second one (SR1) represents attractive short-range interactions involving no ions. The third one (SR2) represents solvation interactions between ions and molecules or between cations and anions. The last term (LR) is the long-range electrostatic interaction contribution.

2.1.1. The Helmholtz energy arising from the repulsive forces. This can be expressed through the improved SRK equation of state given by Wang [8,9]

$$\left(\frac{\Delta A}{RT}\right)_{RF} = \sum_k x_k \ln \frac{x_k RT}{p_0(v-b)}. \tag{2}$$

2.1.2. The Helmholtz energy arising from the attractive forces. This can be expressed through the improved SRK equation of state by Wang [8,9]:

$$\left(\frac{\Delta A}{RT}\right)_{SR1} = \frac{a^{SR}}{bRT} \ln \frac{v}{v+b} \tag{3}$$

$$b = b_m + \sum_{i=ion} x_i b_i \tag{4}$$

b_i is defined by: $\quad b_i = N\pi\sigma_i^3/6 \tag{5}$

where N is Avogadro's number, σ is the hard-sphere diameter, relevant data being shown in table 4. For the molecular mixture, the parameters are calculated using the Wong-Sandler mixing rule [10,11].

$$b_m = \left[\sum_n \sum_m x_n x_m \left(b - \frac{a^{SR}}{RT}\right)_{nm}\right] \bigg/ \left[1 + \left(\frac{A_\infty^E(x)}{RT}\right) - \sum_n x_n \left(\frac{a_n}{b_n RT}\right)\right] \tag{6}$$

$$\left(b - \frac{a^{SR}}{RT}\right)_{nm} = \left[\left(b_n - \left(\frac{a_n^{SR}}{RT}\right)\right) + \left(b_m - \left(\frac{a_m^{SR}}{RT}\right)\right)\right] \bigg/ 2(1 - k_{nm}) \tag{7}$$

where (7) k_{nm} is the binary parameter which can be calculated from critical constants [12]. In equation (6), another term is calculated from

$$\frac{A_\infty^E}{RT} = \sum_n x_n \left(\frac{\sum_m x_m \tau_{nm} g_{nm}}{\sum_m x_m g_{nm}} \right) \tag{8}$$

where (8),

$$g_{nm} = \exp(-0.3\tau_{nm}) \tag{9}$$

the binary parameters τ_{nm} are obtained by fitting gas solubility data at various temperatures and pressures, and these are shown in table 3.

The parameter a^{SR} is calculated as follows,

$$a^{SR} = b_m \left(\sum_n x_n \frac{a_n^{SR}}{b_n} - A_\infty^E(x) \right). \tag{10}$$

The pure molecular components attractive parameter a_n^{SR} is calculated using the expression presented by the improved SRK equation of state by Wang [8,9]

$$a_n^{SR} = 0.42748 \frac{(RT_c)^2}{P_c} \left[1 + m_1(1 - \sqrt{T_r}) + m_2(1 - \sqrt{T_r})^2 + m_3(1 - \sqrt{T_r})^3 \right]^2 \quad \text{for } T_r \leq 1 \tag{11}$$

$$a_n^{SR} = 0.42748 \frac{(RT_c)^2}{p_c} \left[1 + m_1(1 - \sqrt{T_r}) \right]^2 \quad \text{for } T_r > 1 \tag{12}$$

where,

$$m_1 = 0.48344 + 1.58597\omega - 0.3758\omega^2 + 0.23194\omega^3 \tag{13}$$

$$m_2 = 0 \quad (0.35 < \omega \leq 0.56) \tag{14}$$

$$m_2 = 25.689 - 108.63\omega + 150.68\omega^2 - 68.739\omega^3 \quad (\omega > 0.56). \tag{15}$$

for the SO$_2$, DMSO, m_1 is calculated by equation (13). The values of pure molecular component parameters are listed in table 2.

2.1.3. The term of short-range forces to the Helmholtz energy. The third term of the Helmholtz energy expression takes into account interactions between ions and molecules or between cations and anions. This contribution may be considered as the solvation contribution.

$$\left(\frac{\Delta A}{RT} \right)_{SR_2} = \sum_k \sum_l \frac{x_k x_l W_{kl}}{v(1 - \zeta_3)} \tag{16}$$

in which (16), at least one of k and l is an ion, and the packing factor ζ_3 is defined as,

$$\zeta_3 = \frac{N\pi}{6} \sum_k \frac{x_k \sigma_k^3}{v} \tag{17}$$

σ_k is the diameter of a molecular or an ion, the data is shown in table 4, W_{kl} is an adjustable parameter.

2.1.4. The term of long-range forces to the Helmholtz energy. The last term of the Helmholtz energy expression is the long-range electrostatic interaction contribution that is represented with a simplified MSA model proposed by Ball *et al.* [17]:

$$\left(\frac{\Delta A}{RT}\right)_{LR} = -\frac{\alpha_{LR}^2}{4\pi}\sum_i \frac{x_i Z_i^2 \Gamma}{1 + \Gamma\sigma_i} + \frac{v\Gamma^3}{3\pi N} \qquad (18)$$

where the shielding parameter Γ is obtained from the following relations [16]:

$$\Gamma = \frac{\alpha_{LR}}{2}\left[\rho\sum_{j=1}^{c} x_j(z_j + \sigma_j f_j)^2\right]^{1/2} \qquad (19)$$

$$\text{where:} \quad f_j = \frac{\pi C'}{4B'} - \frac{z_j(\alpha_{LR}/2)A' + (\pi\alpha_{LR}A'E')/(12B')}{D'} \qquad (20)$$

$$A' = \left(\rho\sum_{i=1}^{c} x_i z_i^2\right)^{1/2} \qquad (21)$$

$$B' = \left(1 - \frac{\pi}{6}\rho\sum_{i=1}^{c} x_i\sigma_i^3\right) \qquad (22)$$

$$C' = \rho\sum_{i=1}^{c} x_i z_i \sigma_i^2 \qquad (23)$$

$$D' = 1 + \alpha_{LR}\left(\rho\sum_{i=1}^{c} x_i z_i^2 \sigma_i^2\right)^{1/2} \qquad (24)$$

$$E' = \rho\sum_{i=1}^{c} x_i\sigma_i^3 z_i. \qquad (25)$$

Here ρ is number density of total particle in this system, and is defined by:

$$\rho = \rho_m + \rho_i. \qquad (26)$$

Also α_{LR} can be calculated as:

$$\alpha_{LR}^2 = \frac{\varepsilon^2 N}{\varepsilon_0 DRT} \qquad (27)$$

where e is protonic change (1.60219×10^{-19} C); ε_0 is electric perimitivity of freespace (8.45188×10^{-12} J^{-2} C^{-2} m^{-1}). In equation (27), D is dielectric constant of the solution, which takes into account the influence of the ions through Pottel's expression [18]:

$$D = 1 + (D_s - 1)\left(\frac{1 - \zeta_3}{1 + \zeta_3/2}\right) \qquad (28)$$

where D_s is the solvent dielectric constant. In turn this is deduced from the various molecular contributions D_m by

$$D_s = \frac{\sum_m x_m D_m}{\sum_m x_m}.$$
(29)

In equation (28), ξ_3 is defined by equation (17).

Through analysis of the four terms on the RHS of equation (1), only two types of parameters appear in above-mentioned equation, one is a critical parameter and hard-sphere diameter, these being obtained from the literature; another type consists of binary interaction parameters from experimental solubilities. Finally, the calculated parameter is optimized W_{kl} parameters for binary systems.

2.2. *The equations of state of electrolyte solution*

From thermodynamics we have,

$$dA = -SdT - PdV$$
(30)

at constant temperature,

$$P = -\left(\frac{\partial A}{\partial V}\right)_{T,n_k}.$$
(31)

Substituting equation (1) and other expressions in equation (31), the equation of state of electrolyte solution is deduced as

$$\left(\frac{P}{RT}\right) = \left(\frac{P}{RT}\right)_{RF} + \left(\frac{P}{RT}\right)_{SR1} + \left(\frac{P}{RT}\right)_{SR2} + \left(\frac{P}{RT}\right)_{LR}$$
(32)

where

$$\left(\frac{P}{RT}\right)_{RF} = \frac{1}{v-b}$$
(33)

$$\left(\frac{P}{RT}\right)_{SR1} = \frac{a^{SR}}{RTv(v+b)}$$
(34)

$$\left(\frac{P}{RT}\right)_{SR2} = -\sum_k \sum_l \frac{x_k x_l W_{kl}}{v^2(1-\zeta_3)^2}$$
(35)

$$\left(\frac{P}{RT}\right)_{LR} = -\frac{\alpha_{LR}^2}{4\pi D}\left(\frac{\partial D}{\partial V}\right)_{T,n_k} \sum_j \frac{n_j Z_j^2 \Gamma}{1+\Gamma\sigma_j} - \frac{\Gamma^3}{3\pi N}.$$
(36)

For the molecular mixtures, the parameters are calculated using the Wong-Sandler mixing rule.

2.3. *The calculation of gas–liquid phase equilibrium*

On the EOS of the system under consideration, one can write the fugacity coefficient expression given by Prausnitz [19] as:

$$\ln \hat{\phi}_i = \frac{1}{RT} \int_v^{\infty} \left[\left(\frac{\partial P}{\partial n_i} \right)_{T,V,n_j} - \frac{RT}{V} \right] dV - \ln Z. \tag{37}$$

The fugacity coefficient for gas–liquid equilibrium can be calculated by the differential and integral method, further calculating phase equilibrium properties of the electrolyte solution according to the fundamental thermodynamic relationship for gas–liquid equilibrium

$$y_i \hat{\phi}_i^g = x_i \hat{\phi}_i^L \tag{38}$$

where the representation of the component is such that subscript 0 represents SO_2, 1 represents DMSO, 2 represents Mn^{2+}, 3 represents SO_4^{2-}, 4 represents H^+. Therefore the specific expression is:

$$b = b_m + x_2 b_2 + x_3 b_3 + x_4 b_4 \tag{39}$$

where b_m represents the parameter for the molecular mixtures, b_2, b_3, b_4 represents the parameter for the ions in the solution.

The ionic covolumes b_i are deduced from equation (5).

The molecular mixture covolumes b_m can be calculated by:

$$b_m = \left[2x_0 x_1 \left(b - \frac{a}{RT} \right)_{01} + x_0^2 \left(b - \frac{a}{RT} \right)_{00} \right.$$
$$\left. + x_1^2 \left(b - \frac{a}{RT} \right)_{11} \right] \bigg/ \left[1 - \left(x_1 \frac{a_1}{b_1 RT} + x_0 \frac{a_0}{b_0 RT} \right) + \frac{A_\infty^E}{RT} \right] \tag{40}$$

where,

$$\frac{A_\infty^E}{RT} = \frac{x_0(x_0 \tau_{00} g_{00} + x_1 \tau_{10} g_{10})}{x_0 g_{00} + x_1 g_{10}} + \frac{x_1(x_0 \tau_{01} g_{01} + x_1 \tau_{11} g_{11})}{x_0 g_{01} + x_1 g_{11}} \tag{41}$$

due to the binary parameters $g_{ii} = g_{jj} = 1$, $\tau_{ii} = \tau_{jj} = 0$, so equation (41) can be simplified as:

$$\frac{A_\infty^E}{RT} = \frac{x_0 x_1 \tau_{10} g_{10}}{x_0 + x_1 g_{10}} + \frac{x_1 x_0 \tau_{01} g_{01}}{x_0 g_{01} + x_1} \tag{42}$$

g_{nm} can be calculated as equation (9) the parameters of τ_{10} and τ_{01} are obtained by fitting gas solubility data at various temperatures and partial pressures. The regressed binary parameters for the binary systems are listed in table 3, $(b - (a^{SR}/(SR)))_{nm}$ can be calculated as in equation (7). The hard-sphere diameter σ of DMSO is calculated

by Ried [15], $\sigma = 0.809 V_c^{1/3}$, V_c is the critical volume (122.2 cm^3/mol). The calculated result is listed in table 4.

In this system, a_n^{SR} is calculated by:

$$a^{SR} = b_m \left(\frac{x_1 a_1^{SR}}{b_1} + \frac{x_2 a_2^{SR}}{b_2} - A_\infty^E \right) \tag{43}$$

$$\zeta_3 = \frac{N \times 3.14}{6} \frac{x_0 \sigma_0^3 + x_1 \sigma_1^3 + x_2 \sigma_2^3 + x_3 \sigma_3^3 + x_4 \sigma_4^3}{v} \tag{44}$$

while a_{LR} can be calculated as equation (27).

D can be calculated following equation (28) using

$$D_s = \frac{x_0 D_0 + x_1 D_1}{x_0 + x_1}. \tag{45}$$

The dielectric constants for SO$_2$ DMSO are listed in table 5.

This model relates to 5 components of SO$_2$, DMSO, Mn^{2+}, SO$_4^{2-}$, H$^+$, and contains 6 adjustable parameters W_{kl}. As in previous works (Li [20, 21]), in this study we have used a similar approach, ignored the W_{24}, W_{03}, W_{13} parameters because of the well-known charge repulsion effect and because the solvation is generally lower in the case of anions if compared to cations. Hence the model only involved six adjustable parameters W_{cm} and W_{ca} between cation (c) and molecule (m), cation and anion (a).

Furthermore the interaction parameters W_{43} and W_{32} could also be related to σ_c^s and σ_a^p by equation (5) and

$$W_{ca} = \lambda_5 (\sigma_c^5 + \sigma_a^p)^4 + \lambda_6. \tag{46}$$

In these correlations, Stokes diameter σ_c^s for the cations and anionic Pauling diameter σ_a^p for the anions are involved. The values of Pauling and Stokes diameters are listed in table 4. In these correlations the ionic diameters are expressed in Angstroms, the values of coefficients λ_5, λ_6 being -0.03208×10^{-6}, 18.93×10^{-6} respectively, these values were from literature [1]. By equation (46), we can obtain, $W_{43} = -7.92 \times 10^{-4}$ m^3/mol, $W_{32} = -3.85 \times 10^{-4}$ m^3/mol. So experimental data determines four adjustable parameters (table 5).

2.4. *Optimization calculation*

By experimental data correlation, 4 interaction parameters are obtained. They are

$$W_{40} = 0.00152 \, \text{m}^3/\text{mol}, \quad W_{41} = 0.132 \, \text{m}^3/\text{mol}$$
$$W_{20} = -7.63 \, \text{m}^3/\text{mol}, \quad W_{21} = 1.51 \times 10^2 \, \text{m}^3/\text{mol}$$

The comparison between calculated results according to these parameters and experimental data is summarized in table 1. The comparison of SO$_2$ solubilities calculated by the model and experimental data at different SO$_2$ partial pressures are shown in figure 1. Obviously, the solubilities calculated by the model are in good agreement with the experimental data.

Table 1. The comparison of experimental data and calculation values for SO_2 solubilities in mixture absorbent.

									x_{SO_2}	
T (K)	P_{SO_2}, kPa	$x_{H_2SO_4}$	x_{MnSO_4}	x_{DMSO}	y_{SO_2}	y_{O_2}	y_{DMSO}	y_{N_2}	x_{exp}	x_{cal}
294.15	0.228	0.0366	0.00195	0.943	0.00229	0.0776	0.00183	0.918	0.0185	0.0197
294.15	0.306	0.0478	0.00191	0.925	0.00307	0.116	0.00183	0.879	0.0253	0.0238
294.15	0.585	0.0563	0.00187	0.903	0.00585	0.187	0.00182	0.806	0.0387	0.0382
294.15	0.865	0.0644	0.00182	0.882	0.00862	0.257	0.00181	0.733	0.0516	0.0521
294.15	0.956	0.0824	0.00178	0.860	0.00949	0.271	0.00181	0.718	0.056	0.0565
294.15	1.450	0.0975	0.00170	0.821	0.0144	0.321	0.00180	0.663	0.0798	0.0796
294.15	1.945	0.111	0.00162	0.786	0.0194	0.386	0.00180	0.593	0.101	0.102
298.15	0.227	0.0377	0.00195	0.943	0.00228	0.0775	0.00260	0.918	0.0175	0.0185
298.15	0.303	0.0496	0.00191	0.925	0.00304	0.116	0.00260	0.878	0.0238	0.0224
298.15	0.582	0.0575	0.00187	0.904	0.00582	0.186	0.00259	0.805	0.0366	0.0365
298.15	0.861	0.0649	0.00183	0.884	0.00859	0.256	0.00258	0.733	0.0488	0.0497
298.15	0.902	0.1009	0.00175	0.845	0.00859	0.270	0.00256	0.718	0.0519	0.0516
298.15	1.422	0.1141	0.00167	0.810	0.0142	0.320	0.00256	0.663	0.0743	0.0742
298.15	1.941	0.1261	0.00161	0.777	0.0194	0.385	0.00256	0.593	0.0948	0.0949
303.15	0.223	0.0427	0.00194	0.939	0.00223	0.0774	0.00364	0.917	0.0159	0.0171
303.15	0.298	0.0524	0.00191	0.924	0.00297	0.116	0.00362	0.878	0.0217	0.0208
303.15	0.542	0.0705	0.00185	0.895	0.00541	0.186	0.00362	0.805	0.0331	0.0323
303.15	0.787	0.0875	0.00179	0.867	0.00786	0.256	0.00362	0.733	0.0437	0.0431
303.15	0.900	0.1108	0.00174	0.840	0.00893	0.270	0.00361	0.718	0.0472	0.0478
303.15	1.421	0.1229	0.00167	0.808	0.0142	0.320	0.00360	0.662	0.0677	0.0684
303.15	1.943	0.1340	0.00161	0.7769	0.0194	0.385	0.00365	0.592	0.0875	0.0871
308.15	0.186	0.0483	0.00193	0.936	0.00186	0.0771	0.00504	0.916	0.0142	0.0148
308.15	0.290	0.0597	0.00190	0.919	0.00289	0.116	0.00502	0.876	0.0194	0.0193
308.15	0.518	0.0813	0.00183	0.888	0.00517	0.186	0.00503	0.804	0.0294	0.0287
308.15	0.746	0.1014	0.00177	0.858	0.00745	0.256	0.00502	0.732	0.0388	0.0376
308.15	0.895	0.125	0.00172	0.832	0.00889	0.270	0.00502	0.717	0.0419	0.0432
308.15	1.377	0.148	0.00164	0.791	0.0137	0.319	0.00501	0.662	0.0595	0.0599
308.15	1.858	0.169	0.00156	0.754	0.0185	0.384	0.00501	0.592	0.0754	0.0751
313.15	0.182	0.0519	0.00193	0.935	0.00182	0.0769	0.00690	0.914	0.0115	0.0118
313.15	0.271	0.0685	0.00189	0.914	0.00270	0.115	0.00689	0.875	0.0159	0.0154
313.15	0.509	0.0975	0.00181	0.877	0.00507	0.185	0.00689	0.803	0.0236	0.024
313.15	0.719	0.124	0.00174	0.843	0.00718	0.255	0.00689	0.731	0.031	0.0309
313.15	0.798	0.145	0.00169	0.820	0.00794	0.269	0.00687	0.716	0.0336	0.0333
313.15	1.34	0.168	0.00162	0.783	0.0133	0.318	0.00686	0.662	0.0479	0.0481
313.15	1.88	0.189	0.00155	0.749	0.0187	0.383	0.00686	0.591	0.0609	0.0608

Table 2. The values of pure molecular component properties and parameters.

Solvent	DMSO	SO_2
T_c (K)	707 [13,14]	430.8 [15]
P_c (kPa)	5850 [13,14]	7880 [15]
ω	0.414 [13,14]	0.256 [15]
m_1	Calculated by equation (13)	
m_2	0 [15]	− 1.9446 [8]
m_3	0 [15]	15.2851 [15]

Table 3. Optimized τ_{ij} parameters for binary systems.

System	τ_{ij}
SO₂–DMSO	1.85
DMSO–SO₂	−4.35

Table 4. The parameters of substance.

Substance	b_i	Diameter σ, Å	Stocks radius	Pauling radius
SO₂	3.938×10^{-5}	4.112 [15]		
DMSO	8.7055×10^{-5}	5.267 [15]		
H⁺	5.4458×10^{-7}	1.20 [16]	0.73 Å	
Mn²⁺	1.2909×10^{-6}	1.60 [16]	2.48 Å	
SO₄²⁻	2.7771×10^{-5}	4.45 [16]	2.3 Å [22]	2.815 Å [22]

Table 5. The dependence of the dielectric constant of pure substance and temperature.

Substance	Expression	Temperature range, K	Source
SO₂	$D = 36.67 - 0.077T$	287.15–373.15	[23]
DMSO	$D = 91.21 - 0.15T$	293.15–328.15	[23,24]
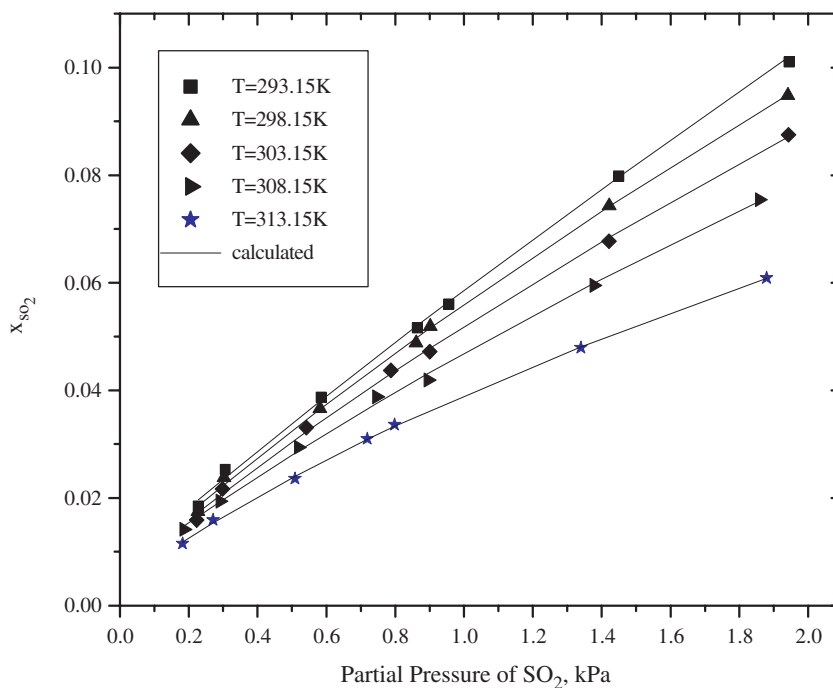
Figure 1. The comparison of experimental data and calculation values for SO₂ solubilities in mixture absorbent at different SO₂ partial pressure.

3. Conclusion

1. According to the measured solubilities of dilute SO_2 in $DMSO + Mn^{2+}$ mixture solvent from 294.15 K to 313.15 K and partial pressure of SO_2 from 0.41 kPa to 2.70 kPA, as well as a previous paper by Furst [1–3,17,20], a suitable electrolyte solution model based on gas–liquid phase equilibrium principles of electrolyte solution has been developed to present a gas–liquid equilibrium system, which takes into account interactions between ions and molecules or between cations and anions to the contribution of the Helmholtz energy, and takes into account the Helmholtz energy arising from the repulsive forces and the attractive forces between molecules through the improved SRK equation of state by Wang *et al.* [7,8].
2. From figure 1, we see that the solubilities calculated by the model are in good agreement with experimental data.
3. Compared with other models, this model is rather simple and applicable; the calculational accuracy is also satisfactory.
4. The experimental solubility and established EOS model in this work can be used as essential data and a model to improve the process design of removal of SO_2 from flue gas.

Nomenclature

A	Helmholtz free energy, $J\,mol^{-1}$
a^{SR}	energy parameter
b	covolume, $m^3\,mol^{-1}$
D	dielectric constant
e	protonic charge, $1.60219 \times 10^{-19}\,C$
g_{nm}	NRTL parameter
k_{ij}	binary parameter for Wong-Sandler mixing rule
N	Avogadro constant, 6.022×10^{23}
$m_1 - m_3$	parameter for equation of state
R	universal gas constant, $8.314\,J\,mol^{-1}\,K^{-1}$
T	temperature, K
p	pressure, kPa
p_c	critical pressure
T_c	critical temperature
x	molar fraction
Z	ionic charge
v	molar volume, $m^3\,mol^{-1}$

Greek letters

Δ	difference
Γ	shielding parameter
σ	hard-sphere diameter
ω	acentric factor
ζ_3	packing factor
ε_0	electric permitivity of free space, $8.854188 \times 10^{-12}\,J^{-2}\,C^{-2}\,m^{-1}$

τ_{ij} NRTL binary parameter

λ correlation parameters defined in equation (46)

Subscripts

a	anion
c	cation
i, j	ionic species
k, l	ionic and molecular species
n, m	molecular property
SR	short-range term
LR	long-range term
0	standard properties

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