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Enhancement of supercritical carbon dioxide solubility models using molecular simulation data

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Abstract−Supercritical carbon dioxide (SC-CO_2) has been used in a broad range of industrial applications due to its unique properties, which underlines the importance of understanding its exact behavior under different operating conditions. In this study, the solubility parameter (SP) of SC-CO_2 was calculated using molecular dynamics simulation at varying temperature and pressure and different concentrations of methanol as a co-solvent. The obtained simulation results were used to create a model for solubility parameter using response surface methodology (RSM). These data were then used to improve three available empirical correlations of SC-CO_2's solubility parameter. The resulting equations were vastly superior in predicting the solubility parameter with an average coefficient of determination of 96.33%.

Keywords: Supercritical Carbon Dioxide, Solubility Parameter, Molecular Dynamics Simulation

INTRODUCTION

Supercritical carbon dioxide is of high importance as an adjustable solvent due to the high diffusion rate and low viscosity [1]. It is widely being used in the extraction process in the industry because of its availability, low toxicity, and low flammability [1,2]. Extraction of essential oils, metal ions, and active ingredients of pharmaceutical plants are some of supercritical carbon dioxide's (SC-CO_2) applications in the industry [3,4].

Solubility, which is one of the important parameters of solvents, specifies its usability for different purposes [5,6]. Pressure and temperature both have considerable impact on the solubility of SC-CO_2 solvent. Moreover, adding co-solvents can increase the solubility by a great extent [7-9]. If the difference between solubility parameter of solute and solvent is high, solute solubility can be increased by reducing temperature, increasing pressure, or adding co-solvents such as methanol, ethanol, and acetone to the SC-CO_2 solvent [9]. Du et al. [1] used molecular dynamics simulation to calculate the solubility parameters of oil molecules and SC-CO_2+co-solvent systems and showed that the solubility parameter is increased by increasing pressure at constant temperature and decreasing temperature at constant pressure. Their findings also indicated that the solubility parameter is proportional to the SC-CO_2 density and that the addition of co-solvents can improve the system's solubility.

If the difference between the solubility parameter of one solute and SC-CO_2 solvent is low, this solute is preferentially dissolved in the SC-CO_2 solvent [9]. When the difference in solubility is about 4 $MPa^{1/2}$, the solute is almost dissolved in the solvent. This rule applies to gaseous, liquid, crystalline, and polymer solutes [10]. Carbon dioxide chemically reacts or interacts with some solvents due to the dispersion forces. Since most gases are non-polar but polarizable, Hildebrand theory of solubility can be used for their dissolution in liquids [8,11]. The solubility parameter is an important constant that can demonstrate the interactions between molecules and is defined as the ratio of square root of cohesion energy to the unit density [12,13]. Eq. (1) shows the definition of Hildebrand solubility parameter [13]:

$$\delta_H = \left(\frac{\Delta H_v - RT}{V_m}\right)^{1/2} = \left(\frac{E}{V_m}\right)^{1/2} \quad (1)$$

where δ_H is the Hildebrand solubility parameter, ΔH_v is the enthalpy of vaporization, E is the molar vaporization energy and V_m is the molar volume. While the Eq. (1) can be used to predict the liquids' solubility parameter near their boiling points with acceptable accuracy, it cannot be used to determine the solubility of supercritical carbon dioxide as the vaporization enthalpy is meaningless in supercritical conditions [8,10]. To solve this issue, Hansen et al. [14] proposed a three-dimensional solubility parameter (Eq. (2)):

$$\delta^2 = \delta_d^2 + \delta_p^2 + \delta_h^2 \quad (2)$$

where δ_d is the solubility parameter of dispersion forces, δ_p is the solubility parameter of the polar intermolecular forces, and δ_h is the solubility parameter related to the energy of hydrogen bonds. Furthermore, Giddings et al. [15] proposed an empirical correlation as a function of pressure and density to calculate the solubility parameter of supercritical fluids (Eq. (3)). Then, Marcus et al. [10] modified Eq. (3) by introducing reduced temperature (Eq. (4)). Later, Zhang et al. [9] further improved Marcus equation by adding reduced pressure (Eq. (5)).

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$$\delta = 3.02 P_c^{1/2} \rho_r \quad (3)$$

$$\delta = 2.79 P_c^{1/2} \rho_r T_r^{1/4} \rho_r \quad (4)$$

$$\delta = \frac{2.79 P_c^{1/2} T_r^{1/4}}{P_r^{1/8}} \rho_r \quad (5)$$

The solubility parameter of a solvent can be determined using measurement, empirical correlations, and molecular simulations [10,16]. However, due to the high cost and difficulty of experimental methods to calculate the solubility parameter, molecular dynamics simulation has gained researchers' attention. In recent years, molecular dynamics simulation has been extensively used to calculate diffusion coefficients, adsorption isotherms, and solubility parameters [17-21].

In this study, molecular dynamics simulation was used to compute the solubility parameter of supercritical carbon dioxide at various temperatures and pressures in the presence of methanol. To validate the simulation results, the solubility parameter of supercritical CO_2 was first calculated at 318 K and 8.5-40 MPa, and also 363.15 K and 70 MPa at methanol concentration of 0-0.3, and then the results were compared with experimental data [3,22] and previous simulation results [1,9]. Then, the solubility parameter was modeled with response surface methodology and was compared with the previous studies. Finally, a model was proposed for the anticipation of supercritical carbon dioxide solubility parameter using molecular simulation results and the three temperature and pressure dependent empirical relations (Eqs. (3)-(5)).

SIMULATION DETAILS

In this work, all the simulations were carried out using BIOVIA Materials Studio 2017 software package. In all the simulations, COMPASS force field [1,9] was used for molecular interactions alongside Ewald and Atom-based summation methods for electrostatic and van der Waals interactions, respectively, with cut off distance of 12.5 Å. Positioning of the carbon dioxide and methanol molecules in the simulation cell was optimized with Forcite module to give the most stable structure. Subsequently, the Amorphous cell module was used to apply periodic boundary conditions at specified temperature [23]. As shown in Table 1, the total number of molecules used in the simulation was constant and equal to 512. Geometry optimization was used to yield an amorphous cell with lowest level of energy. In the end, the system was equilibrated in NVT ensemble for 20 ps (timesteps of 1 fs) to reach the desired temperature using Nose thermostat. Results of the simulation were compared to the experimental data using coefficient of determination (R^2) (Eq. (6)) and root-mean-square error (RMSE) (Eq. (7)):

Table 1. Molecular composition of CO_2 and CO_2+methanol systems

Concentration of co-solvent (%)	Number of molecules		
	CO_2	Methanol	Total
0	512	0	512
5	484	28	512
10	461	51	512
16	430	82	512
20	410	102	512
25	384	128	512
30	358	154	512

$$R^2 = 1 - \frac{\Sigma_{i=1}^{n} (\delta_i^{exp} - \delta_i^{sim})^2}{\Sigma_{i=1}^{n} (\delta_i^{exp} - \delta_m^{exp})^2} \quad (6)$$

$$RMSE = \sqrt{\frac{\Sigma_{i=1}^{n} (\delta_i^{exp} - \delta_i^{sim})^2}{n}} \quad (7)$$

where n is the number of data, δ_i^{exp} is the experimental solubility parameter, δ_i^{sim} is the simulated solubility parameter, and δ_m^{exp} is the average experimental solubility parameter. To calculate the coefficient of determination and root-mean-square error for the response surface method and the third model, the solubility parameter derived from the molecular simulations replaces the experimental solubility parameter.

To validate the results of the molecular dynamics simulation, solubility parameters of SC-CO_2 and SC-CO_2-methanol solvents at different temperatures and pressures were compared with experimental data [3,22] and Du et al's [1] and Zhang et al's [9] simulations. Table 2 shows the values of determined solubility parameter from this study, experimental results, and Du et al. [1] and Zhang et al. [9] simulations. As shown in Table 2, simulated solubility parameters are in good agreement with the experimental data, except at 8.5 MPa (that has an error of 11.4%). This is evident in

Table 2. Solubility parameter of pure SC-CO_2 solvent from MD simulations and experimental data at 318 K [3]

P (MPa)	δ_{exp} $(MPa)^{1/2}$ [3]	δ_{sim} $(MPa)^{1/2}$ [9]	δ_{sim} $(MPa)^{1/2}$ [1]	δ_{sim} $(MPa)^{1/2}$ This work	Devi. % [9]	Devi. % [1]	Devi. % This work
8.5	4.9	4.78	-	4.341	2.45	-	11.4
10	7.7	7.64	8.637	7.810	0.78	12.169	1.41
20	14.3	12.57	13.157	14.444	12.10	7.993	1.01
25	15.0	13.34	14.593	15.163	11.07	2.713	1.09
30	15.6	13.70	15.105	15.451	12.18	3.173	0.96
40	16.4	14.67	15.765	16.016	10.55	3.871	2.34
Average Devi. %					**8.19**	**5.98**	**3.04**
RMSE					**1.4358**	**0.7069**	**0.3004**

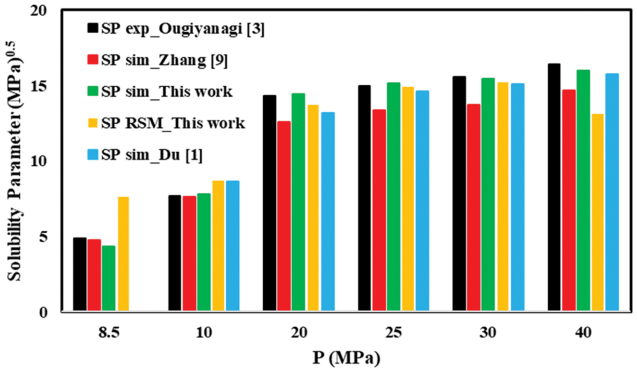

Fig. 1. Solubility parameter of SC-CO_2 from experimental data, design of experiment model, this work's simulation, and Du et al. [1] and Zhang et al. [9] simulations.

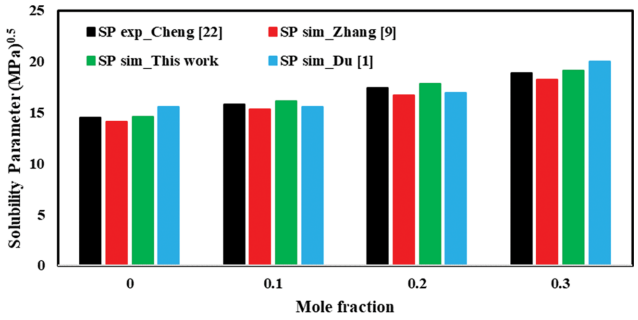

Fig. 2. Solubility parameter of SC-CO_2-Methanol solvent from experimental data (black) and simulation results of this work (green), Zhang et al. [9] (red), and Du et al. [1] (blue).

the values of average deviation and RMSE that are equal to 3.04% and 0.3004, respectively. In comparison to Du et al. [1] and Zhang et al. [9] studies, the average deviations for the solubility parameter of SC-CO_2 solvent were 5.98% and 8.19%, respectively. Fig. 1 shows the solubility parameter of SC-CO_2 solvent for experimental data [3], design of experiment model, this study's simulation results, and Du et al. [1] and Zhang et al. [9] simulations versus pressure at 318 K.

Simulated and experimental solubility parameter of SC-CO_2-methanol solvent at 363.15 K and 70 MPa is given in Table 3. Average deviation for the simulation of SC-CO_2-methanol solvent was calculated to be 1.56%, whereas this error was 4.31% and 3.41% for Du et al. [1] and Zhang et al. [9] simulations, respectively. As demonstrated in Table 3, the results of this simulation were more accurate than the results of Du et al. [1] and Zhang et al. [9]. For this solvent, unlike the pure SC-CO_2, the results of the Zhang et al. [9] simulation were more consistent with the experimental data compared to the results of Du et al. [1]. Fig. 2 shows the variation of SC-CO_2-methanol's solubility parameter with mole fraction for experimental data [22], this study's simulation, Du et al. [1] and Zhang et al. [9] simulations at 363.15 K, 70 MPa, and methanol's mole fraction of 0 to 0.3.

After comparing the solubility parameter derived from molecular dynamics simulation in this study with other simulation results and experimental data, it can be concluded that this study's simulation yielded more accurate results that can be used for response surface methodology modeling of the solubility parameter.

Table 4 shows a comparison between the molecular dynamics simulation carried out in this study and simulations of Du et al. [1] and Zhang et al. [9] to contrast the different procedures used in the simulations. As can be seen in Table 4, all the simulations were carried out in Materials Studio software with COMPASS force field. In this study, Ewald and atom-based summation methods were used for electrostatic and van der Waals interactions, respectively, while the other two simulations used group-based summation method. The Ewald method is an accurate and fast-converging method for calcuation of interactions. In the Ewald method, the space of the simulation is divided into the short range and long range. Interactions in the short range are calculated in real space, whereas the interactions in the long range are calculated using Fourier transforms, which reduces the calculation time significantly while preserving the accuracy of the calculations [24]. The duration of the simulation in this study was 20 ps in total (excluding the time spent for the construction of amorphous cell in the NPT ensemble to calculate its density) with the timestep of 1fs. In Du et al's [1], and Zhang et al's [9] works, however, the simulations were run for 500 ps and 200 ps, respectively, with the timesteps of 1 fs. In this work and the work of Zhang et al. [9], NVT ensemble was used for equilibration, while Du et al. [1] reported using NPT ensemble. Moreover, Nose, Berendsen, and Andersen thermostats were

Table 3. Solubility parameter of SC-CO_2-Methanol solvent from MD simulations and experimental data at 363.15 K and 70 MPa [22]

Mole fraction	δ_{exp} (MPa)$^{1/2}$ [22]	δ_{sim} (MPa)$^{1/2}$ [9]	δ_{sim} (MPa)$^{1/2}$ [1]	δ_{sim} (MPa)$^{1/2}$ This work	Devi. % [9]	Devi. % [1]	Devi. % This work
0	14.5	14.1	15.554	14.596	2.76	7.270	0.66
0.05	-	-	-	14.772			
0.1	15.8	15.3	15.554	16.150	3.16	1.556	2.22
0.16	-	-	-	16.775			
0.2	17.4	16.7	16.920	17.775	4.02	2.758	2.16
0.25	-	-	-	18.193			
0.3	18.9	18.2	19.968	19.128	3.70	5.651	1.21
Average Devi. %					**3.41**	**4.31**	**1.56**
RMSE					**0.5895**	**0.7973**	**0.2847**

Table 4. Comparison of simulation details in this study with Du et al. [1] and Zhang et al. [9]

	Du et al. [1]	Zhang et al. [9]	This work
Software	Materials studio	Materials studio	Materials studio
Force Field	COMPASS	COMPASS	COMPASS
Summation method			
Electrostatic	Group-based	Group-based	Ewald
Van der Waals	Group-based	Group-based	Atom-based
Time step	1 fs	1 fs	1 fs
Total simulation time	500 ps	200 ps	20 ps (NVT)+50 ps (NPT)
Ensemble	NPT	NVT	NVT
Thermostat	Andersen	Berendsen	Nose

used to control the temperature in this study, Du et al's [1], and Zhang et al's [9] simulations, respectively. Shahamat et al. [24] used Nose and velocity-rescaling thermostats for calculating polymer/solvent solubility parameter and showed that these thermostats produce similar results.

RESPONSE SURFACE METHODOLOGY

Other than temperatue and pressure, the solubility parameter of SC-CO_2 is also dependent on the mole fraction of the co-solvent [9]. According to the literature, modifiying the temperature and pressure alone cannot increase the solubility parameter of supercritical carbon dioxide to infinity [25]. In this study, Box-Behnken Design method was used as one of the response surface methods to optimize the solubility parameter. The design of experiment consisted of 15 runs and three central design points. Central points are used to increase the reliability and reproducibility of the results. In this study, temperature, pressure, and methanol mole fraction were used in three levels as the inputs of the design of the experiment, and the solubility parameter of the SC-CO_2 was used as the output (response). Ranges and levels of the independent variables and all the 15 runs of the design of the experiment are shown in Table 5 and Table 6, respectively. Predicted parameters of solubility from molecular dynamics simulation and design of experiment are shown in Table 8. To model the system, the following polynomial equation was used to fit the SC-CO_2 solubility parameter (Eq. (8)):

$$Y = b_0 + \sum_{i=1}^{n} b_i x_i + \sum_{i=1}^{n}\sum_{j=1}^{n} b_{ij} x_i x_j + \sum_{i=1}^{n}\sum_{j=1}^{n} b_{ii} x_i^2 + \varepsilon \quad (8)$$

where b_0 is a constant, b_i is the variable slope of x_i (i=1, 2, 3), b_{ij} is the reciprocal interaction term between x_i and x_j (i, j=1, 2, 3), and b_{ii} is the second degree curvature term of x_i, and ε is the remaining term.

Regression and analysis of the experimental data were carried out in Minitab 2017 software. Analysis of variance (ANOVA) was used to determine the significance of each term in the equation and a second degree polynomial was fitted to the data, yielding a correlation between independent variables and the response (Eq. (9)).

$$SP = 224 - 14.7x - 1.111T - 1.187P - 23.3x^2 + 0.00128T^2 - 0.01769P^2 + 0.117xT - 0.035xP + 0.00698TP \quad (9)$$

Table 5. Ranges and levels of the variables used in the RSM design of experiment

Variables	Ranges and levels		
Mole fraction (x)	0	0.15	0.3
Temperature (T (K))	298	323	348
Pressure (P (MPa))	7	20	33

Table 6. RSM (this work)

x	T (K)	P (MPa)	δ_{sim} $(MPa)^{1/2}$ This work	δ_{RSM} $(MPa)^{1/2}$ This work
0	298	20	16.053	17.37592
0	323	7	4.056	5.29409
0	323	33	15.677	14.65253
0	348	20	10.051	10.14992
0.15	298	7	15.826	14.53447
0.15	298	33	18.182	19.21031
0.15	323	20	15.193	15.917
0.15	323	20	15.125	15.917
0.15	323	20	15.763	15.917
0.15	348	7	3.621	3.70747
0.15	348	33	15.048	17.45731
0.3	298	20	20.342	21.05872
0.3	323	7	8.153	9.99089
0.3	323	33	19.499	19.07633
0.3	348	20	16.095	15.58772

Table 7. Response surface regression: SP versus x, T (K), and P (Mpa)

Term	Coded coefficients	T-value	P-value
Constant	15.360	15.49	0.000
x	2.281	3.76	0.013
T	−3.199	−5.27	0.003
P	4.594	7.56	0.001
x*x	−0.524	−0.59	0.583
T*T	0.799	0.89	0.412
P*P	−2.990	−3.34	0.020
x*T	0.439	0.51	0.0631
x*P	−0.069	−0.08	0.939
T*P	2.268	2.64	0.046

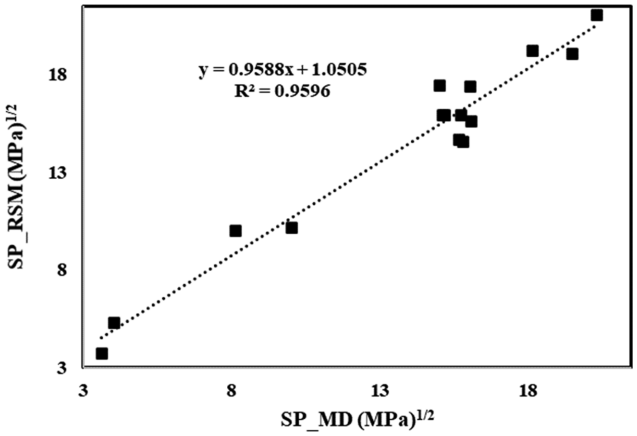

Fig. 3. Accuracy of RSM model in prediction of molecular simulation results.

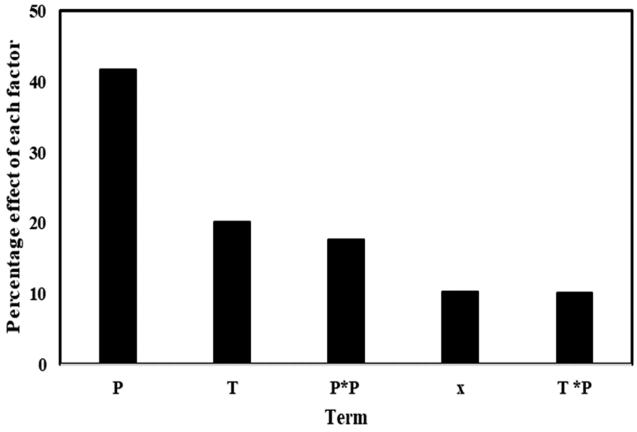

Fig. 4. Significance of each term in the response surface modeling of solubility parameter.

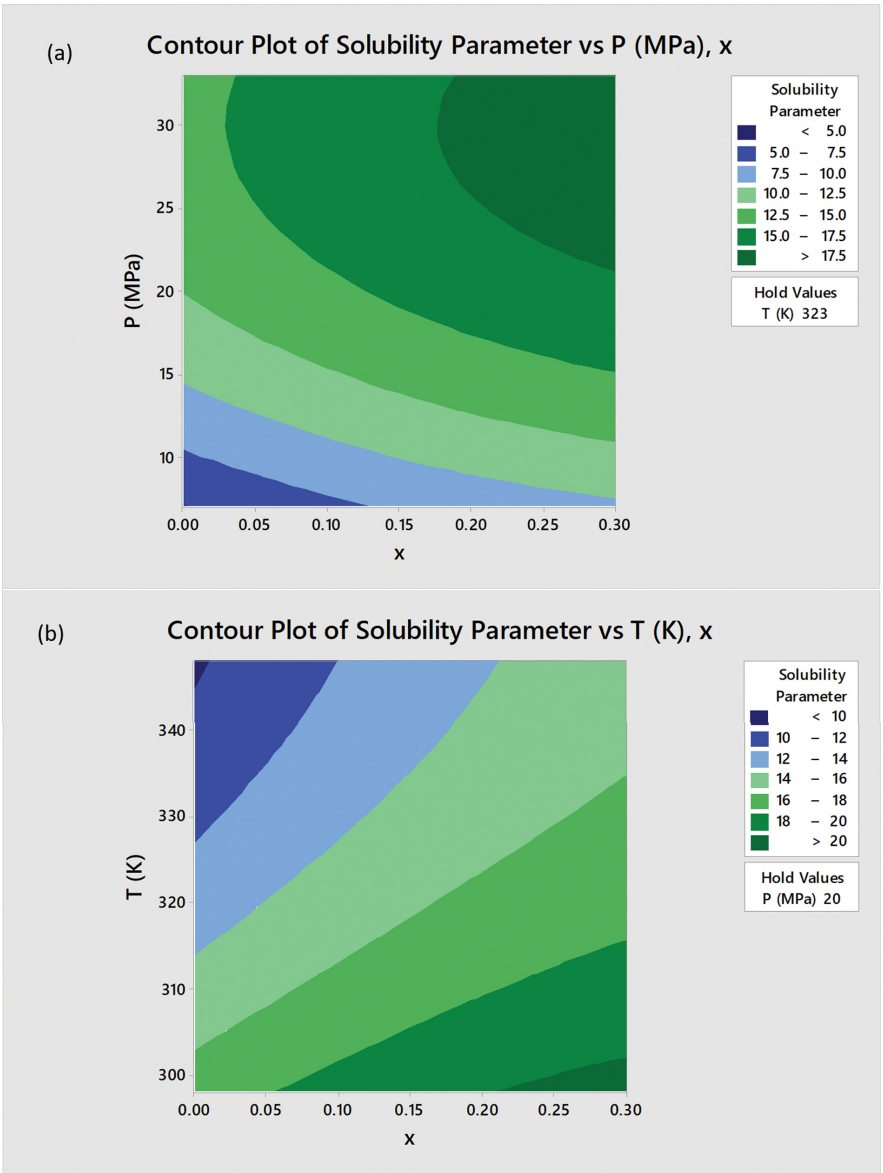

Fig. 5. Contour plots of SC-CO_2 solubility parameter at constant temperature of 323 K (a), and constant pressure of 20 Mpa (b).

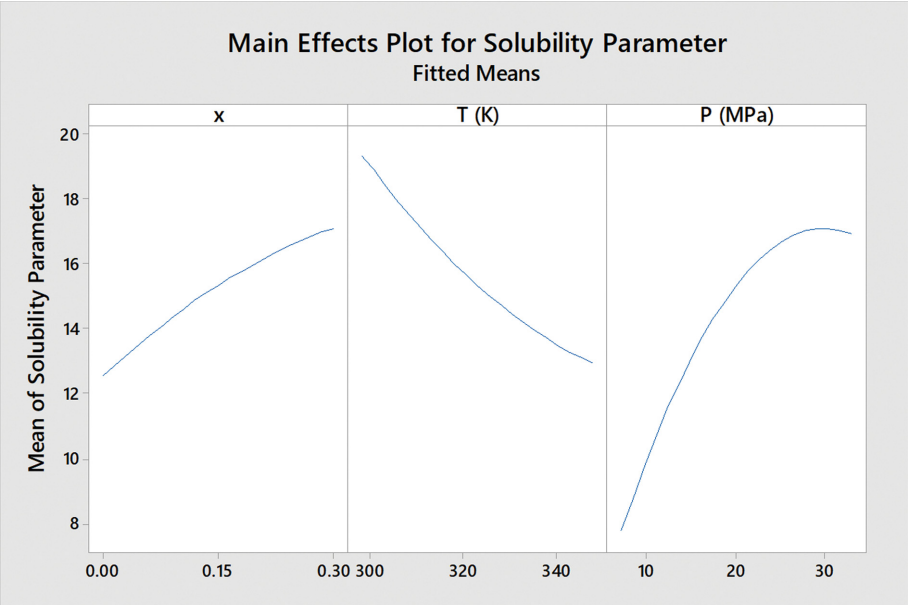

Fig. 6. Impact of changing temperature, pressure, and methanol mole fraction on the solubility parameter of SC-CO_2.

The correlation coefficient (R^2) is a quantitative test for evaluating the relation between the experimental data (simulation data in here) and the predicted values. By comparing the solubility parameter derived from the molecular dynamics simulation and the predicted ones from response surface method, it was found that they were reasonably consistent in the range of the experiment with R^2=95.96%. Regression parameters are shown along with the analysis of variance (ANOVA) in Table 7. According to the R-squared test, it can be concluded that the second-degree polynomial is a good fit for this model and can explain the behavior of the response surface.

P-values (Table 7) have an important role in assessing the interaction effects of independent variables and determination of each term's significance. The lower the P-value is, the higher its impact is on the response surface. Fig. 3 shows a comparison between simulated solubility parameters and predicted solubility parameters from response surface method, which shows a coefficient of determination of 95.96%. To have a better understanding of the results, Pareto analysis was used to calculate each parameter's influence on the response. Pareto analysis is as shown below:

$$P_i=\left(\frac{b_i^2}{\Sigma_{i=1}^{n} b_i^2}\right)\times 100 \quad i\neq 0 \tag{10}$$

where b_i represents the second-degree polynomial coefficient. As can be seen in Fig. 4, the most influential factors on the SC-CO_2 solubility parameter are pressure (41.69%), temperature (20.24%), second power of pressure (17.65%), methanol mole fraction (10.28%), and temperature-pressure interaction term (10.16%). Temperature has a negative effect, while pressure and methanol concentration have a positive effect on the solubility parameter of SC-CO_2. The interaction term's effect was also remarkable, causing a decrease in solubility parameter by raising temperature and reducing pressure.

Fig. 5 shows a two-dimensional contour plot of SC-CO_2 solubility parameter. According to Fig. 5(a), at constant temperature of 323 K, the parameter of SC-CO_2 increases with pressure and methanol concentration, giving the highest value of solubility parameter at P=33 MPa and x=0.3, equal to 17.5 $(Mpa)^{0.5}$. Addition of methanol to the SC-CO_2 system improves the solubility of the solvent by increasing the polarity of the system and intensifying the molecular interaction. Moreover, increasing the pressure dampens the effect of hydrogen bonds on methanol molecules and leads to a better and more uniform dispersal of methanol molecules in the system [9]. The findings of this work and prior studies confirm that adding methanol to the SC-CO_2 solvent will increase its solubility parameter quite considerably [25,26].

In Fig. 5(b), where the pressure is constant at 20 Mpa, increasing the methanol concentration and decreasing the temperature will increase the solubility parameter. The highest solubility parameter in this plot is 20 $(Mpa)^{0.5}$, which is at 298 K and methanol mole fraction of 0.3. The negative effect of temperature on the solubility parameter is also evident in Fig. 6.

COMPARISON OF RESPONSE SURFACE METHODS AND MODELS OF PRIOR STUDIES

In this study, the results of the surface response model (Table 6) were compared with Eqs. (3)-(5). Table 8 shows the coefficient of determination and root-mean-square error for the response surface model and Eqs. (3)-(5). According to Table 8, the Giddings et al. model [15] had a coefficient of determination of 94.199%, which was the highest after the response surface model (R^2=95.96%). Consequently, Eqs. (3)-(5) were modified with molecular dynamics simulation data, resulting in the enhanced Eqs. (11)-(15) listed in Table 9. Another equation was also created by averaging the three modified equations (Eq. (14)). The dataset used for modifying the equations was obtained from 63 molecular simulations at three levels of temperature (298, 323, 348 K), three levels of pressure (7, 20, 33 Mpa), and seven levels of methanol mole fraction (0, 0.05,

Table 8. Coefficient of determination and RMSE for response surface method and Eqs. (3)-(5) (the inputs are taken from Table 6)

Model	RMSE	R^2%
RSM	1.107029	95.96
Eq. (3)	1.364068	94.199
Eq. (4)	2.042075	84.7573
Eq. (5)	2.794714	66.7718

Table 9. Enhanced equations from 63 simulation data

$$\delta = 3.33979 P_c^{1/2} \rho_r^{0.7605354} \quad (11)$$

$$\delta = 3.419897 P_c^{1/2} T_r^{1/4} \rho_r^{0.7879373} \quad (12)$$

$$\delta = \frac{3.421028 P_c^{1/2} T_r^{1/4}}{P_r^{0.0014735}} \rho_r^{0.7890034} \quad (13)$$

$$\delta = 1.1311905 P_c^{1/2} \rho_r^{0.779158} \left(1 + T_r^{1/4} + \frac{T_r^{1/4}}{P_r^{0.0014735}} \right) \quad (14)$$

Table 10. Comparison of the results of Eqs. (3)-(5), Eqs. (11)-(14), and response surface method

	RMSE	R^2%	RMSE	R^2%
			Corrected (Eqs. (11)-(14))	
RSM	1.839998	88.019	-	-
Model 1 (Eq. (3))	1.423620	94.579	1.073994	96.033
Model 2 (Eq. (4))	2.060691	86.465	1.010889	96.479
Model 3 (Eq. (5))	2.807787	74.044	1.010880	96.480
Sum models	-	-	1.018156	96.375

0.1, 0.15, 0.2, 0.25, 0.3). Table 10 shows the coefficient of determination and root-mean-square error for the response surface model of the 63 aforementioned simulation data, Eqs. (3)-(5), and Eqs. (11)-(14). For this dataset, Giddings et al. model [15] had the highest accuracy with R^2=94.579% whereas Zhang et al's model had the lowest fit with R^2=74.044%. Modified equations, however, had a high accuracy of about 96%. Eq. (14) was also very accurate with R^2=96.375%.

CONCLUSION

The effect of temperature, pressure, and methanol mole fraction on the solubility parameter of SC-CO_2 was investigated via molecular dynamics simulation. The average deviation of the simulation's results from the experimental data was 1.56% and the root-mean-square error was 0.2847, which proved the accuracy of the simulations. The observations show that the solubility parameter increases when the pressure or methanol concentration is increased, while it decreases when the temperature is increased. To formulate the effect of all these changes, response surface methodology was used to model the solubility parameter as a function of temperature, pressure, and methanol mole fraction. This information was then used to improve the accuracy of three existing equations for the solubility parameter of supercritical CO_2. The improved equations were able to predict the simulated solubility parameter of SC-CO_2 with considerably less error.

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