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Solubility estimations for Disperse Blue 14 in supercritical carbon dioxide

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Abstract

Supercritical carbon dioxide is an alternative solvent that is considered for dry dyeing processes in the textile industry. The application of this process requires a study to determine the dye solubility in supercritical carbon dioxide. The solubility in supercritical carbon dioxide of a disperse dye at temperatures of 40, 60 and 80 °C and pressures from 100 to 350 bar was evaluated in a previous study. In the work described here, these solubility values have been correlated with fairly good accuracy using a model based on thermodynamic aspects and the use of equations of state. Physical properties and critical parameters of the solid have been estimated using different group contribution methods. The thermodynamic model has been developed by means of a program based on fitting the solid sublimation pressure and binary interaction parameter. The results obtained in the solubility correlation show that the choice of group contribution method is more important than the choice of equation of state.

Keywords: Equation of state; Group contribution method; Critical properties; Fluid–solid equilibrium; Estimation; Disperse dye

1. Introduction

The textile industry uses large amounts of water in its dyeing processes. Due to environmental problems such as the emission of organic materials in wastewater, a new dyeing process has been developed in which supercritical carbon dioxide is used as the solvent for dyes. The advantages of supercritical carbon dioxide are that it can be recycled, is low in cost, non-toxic and non-flammable. Moreover, the dyes can be more efficiently utilized because all the dyes dissolved in the supercritical fluid can be recovered when the fluid is expanded. Last year, many authors have investigated supercritical dyeing technology [1–13].

However, a crucial property for the design of several processes with supercritical solvents is the solubility of the substances treated in a supercritical fluid. The solubilities of many dyes have been measured by different investigators [14–28]. In addition, the design and development of processes with supercritical fluids depend on the ease of modelling and predicting the phase equilibrium as exactly as possible – in this case, the supercritical fluid–solid equilibrium. Fluid–solid thermodynamic modelling presents difficult mathematical challenges, even when it is possible to obtain the experimental solubility data of the solute in the supercritical fluid. In most cases, it is necessary to introduce additional adjustment parameters. Furthermore, given the lack of thermodynamic data for the substances involved, it would also be necessary to estimate parameters that cannot be determined empirically.

Very few studies have been published on the correlation of equilibrium data for this type of system.

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Lee et al. [16] correlated the solubility of two disperse dyes, C.I. Disperse Blue 3 and C.I. Disperse Blue 79, in supercritical carbon dioxide using the expanded liquid model in which the supercritical fluid phase was considered as the expanded liquid. In this way, a binary interaction parameter was obtained by regression of the experimental data and this was found to be almost independent of temperature and strongly dependent on the density of carbon dioxide.

In the work published by Mishima et al. [20], the solubilities of azobenzene, *p*-hydroxyazobenzene, *p*-dimethylaminoazobenzene and anthraquinone were measured in SC-CO_2 at 308.2, 318.2 and 333.2 K over the pressure range 9.1–25.3 MPa using a flow-type apparatus. The solubilities of azo and anthraquinone dyes were correlated by the Soave–Redlich–Kwong equation of state (EOS) with conventional mixing rules. Furthermore, the two binary parameters required in the EOS (l_{ij} and k_{ij}) to give the best fit with the experimental solubility data were correlated using pure-component properties for these substances. The critical temperature and pressure were estimated by the Lydersen group contribution method.

Ferri et al. [29] correlated the solubilities of 16 compounds with five literature equations as well as with a newly proposed semiempirical equation. From the literature correlation, the Chrastil equation gave the best results in relation to the number of fitting parameters involved. The new correlation was successfully applied and the agreement with experimental data was found to improve if fusion properties of the solute were experimentally measured. Moreover, the use of the new correlation is recommended when data with high experimental accuracy are available. The application of this method requires greater effort because the knowledge of some dye physical properties is necessary. However, if these properties are experimentally measured then the results justify this choice of approach.

Tamura and Shinoda [30] used the Peng–Robinson, Peng–Robinson–Stryjek–Vera (PRSV), and a modified form of PRSV EOS to represent the binary and ternary solubilities of the dyes C.I. Disperse Blue 134 and C.I. Disperse Yellow 16 in supercritical conditions. The modified form of PRSV EOS proposed in their previous work takes into account the temperature dependence of a pure characteristic parameter in the PRSV EOS. The critical constants and acentric factor of pure components used in the EOSs were estimated by group contribution methods. The critical properties were estimated by the Miller method, and the acentric factor and vapour pressure of the dye were evaluated using the Lee–Kesler method. The method developed by Miller is derived from Lydersen's method. However, the Lee–Kesler method for estimating sublimation pressure involves the use of the normal boiling point and the critical point to obtain a generalised constant in the Clapeyron equation. In this way, the data obtained for the pressures would correspond to the liquid–gas equilibrium curve. These data are vapour pressure and not sublimation pressure data.

Joung et al. [31] measured the solubility of Disperse Blue 14 (the dye studied in this work). Also, the data were modelled by an empirical density correlation and a quantitative equation of state proposed by these authors and based on nonrandom lattice theory. They employed group contribution methods to estimate the necessary physical properties. Lydersen–Forman–Thodos's method [39] was used for boiling point and critical temperature, Miller's method [39] for critical pressure, and vapour pressure was estimated by Lee–Kesler correlation. They concluded that both models calculated the solubility of dye reasonably well.

2. Thermodynamic model

The use of an equation of state has been one of the most extensively applied methods to predict phase equilibria at high pressures. The method associates an equation of state with a mixing rule based on the thermodynamic equilibrium conditions. In the work described here, the phase-equilibrium data are modelled with the Redlich–Kwong (RK), Soave–Redlich–Kwong (SRK) and Peng–Robinson (PR) equations of state [32]. The latter equation of state is used in most of the studies published in the literature. The following mixing rules are used:

$$a = \sum_i \sum_j y_i y_j a_{ij} \tag{1}$$

$$b = \sum_i y_i b_{ii} \tag{2}$$

$$a_{ij} = \left(1 - k_{ij}\right)\sqrt{a_i a_j} \tag{3}$$

where k_{ij} is a mixture interaction parameter determined by fitting P–y data, a_{ii} and b_{ii} are pure-component parameters defined by each equation of state and y_i is the mole fraction of component *i*.

The method for modelling equilibrium data involved calculating the fugacity of the components in the different phases and making them equal. In this way, the solubility of the solid solute (2) in the supercritical fluid (1) can be calculated by means of Eq. (4), which considers a solid phase – composed of the pure solute (2) – in equilibrium with a fluid phase formed by a mixture of solvent (1) and solute (2) [32].

$$y_2 = \frac{P_2^{\text{sat}}}{\hat{\phi}_2^{\text{F}} P} \exp \frac{\left(P - P_2^{\text{sat}}\right) v_2^{\text{S}}}{RT} \tag{4}$$

The calculation of the solubility y_2 therefore requires a knowledge of P_2^{sat}, υ_2^{S} and an equation of state (with its associated mixing rules) for the calculation of $\hat{\phi}_2^{\mathrm{F}}$. The fugacity coefficient is the property calculated by a thermodynamic model. The other properties of the solid (P_2^{sat} and υ_2^{S}) should be obtained from independent sources.

There are many properties that affect the results of calculations of solid solubilities in supercritical carbon dioxide using an equation of state and mixing rules. Besides the critical constant, the sublimation pressures of solids also play a dominant role in terms of the calculation results. The sublimation pressure of a high molecular weight compound is too small for accurate experimental measurement. Cortesi et al. [33], Huang et al. [34], Kraska et al. [35] and Reverchon et al. [36] suggested that the sublimation vapour pressure should be considered as an adjustable parameter.

In a previous study [37], RK, SRK and PR EOS with Lorentz–Berthelot (LB) mixing rules (MR) were used to calculate the fugacity coefficient. In order to calculate this coefficient, a binary interaction parameter k_{ij} was obtained by fitting the experimental solubility data. The acentric factor (ω) was calculated by Lee–Kesler correlation [38]. The solid molar volume was calculated using the Immirzi and Perini group contribution method [39]. Lydersen's [40] and Fedors' [41] group contribution methods were used to estimate the critical pressure, critical volume and critical temperature of Disperse Blue 14.

In this work, several group contribution methods (GCM) for normal boiling point, critical temperature and critical pressure of the solid were used to analyse the applicability of this correlation method and to study the influence of each parameter. Critical parameters were estimated using Ambrose [42,43], Constantinou–Gani [44,45], Klincewicz–Reid [46], Lydersen [40,47], Joback [41,48,49] and Somayajulu [50] group contribution methods with Joback and Meissner boiling temperature estimation methods [39–41]. Furthermore, the quadratic van der Waals fluid mixing rules (VDW) [32] for the energy parameter were employed with one interaction parameter (k_{ij}) in the corresponding combining rules. The value of k_{ij} obtained by correlating fluid–solid equilibrium data can have either a positive or a negative value. Several limitations have been reported on using this fitting parameter [51]:

- k_{ij} should be regressed from experimental data and are a function of temperature.
- Several researchers [52,53] noticed that the k_{ij} values obtained from regression of experimental equilibrium data do not seem to follow certain general trends. Thus, the development of generalised correlations using solid properties as adjustable parameters is difficult but is still an open area for investigation.
- The interaction parameters often include the possible errors in the thermophysical properties of the solid (vapour pressures and critical properties).

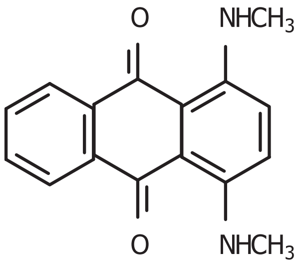

Fig. 1. Structure of Disperse Blue 14.

Coutsikos et al. [51] concluded that cubic EOS with the VDW mixing rules are useful for correlating and extrapolating experimental data but not for prediction purposes.

Therefore, if the sublimation pressure is measured or estimated and the interaction parameter is a constant that is independent of temperature, the use of a cubic EOS is a thermodynamically rigorous procedure. In this work, the use of such a model is an empirical computational procedure.

As described previously, two parameters in this model – k_{12} and the solid sublimation pressure (P_2^{sat}) – were fitted by minimizing the error (average absolute relative deviation, AARD) between experimental and calculated solubility data.

This thermodynamic model was developed using a Visual Basic® Program based on the fitting of these parameters – although it is clearly useful when both parameters are known. The developed program can be used for any fluid–solid equilibrium [54].

3. Experimental solubility data

The solute under investigation was 1,4-dimethylamino-anthraquinone (Disperse Blue 14) ($C_{16}H_{14}N_2O_2$, 266.3 g/mol) (see Fig. 1). The solubility data for Disperse Blue 14/CO_2 were determined in a previous study [37].

Table 1
Critical properties of Disperse Blue 14 obtained using different combinations of group contribution methods

Combination of GCM	Disperse Blue 14	
	T_c (K)	P_c (bar)
Ambrose + Meissner	792.81	20.86
Constantinou–Gani	799.82	24.03
Joback	1137.62	27.18
Klincewicz + Meissner	873.12	23.34
Lydersen + Meissner	790.02	24.60
Somayajulu + Meissner	785.36	24.10

Table 2
Results of the modelling of the Disperse Blue 14/CO_2 phase equilibrium with the RK EOS and the VDW MR

GCM-T	k_{12}	AARD (%)	P_2^{sat} (bar)	GCM-T	k_{12}	AARD (%)	P_2^{sat} (bar)
Amb + Meis-40	−0.594	31.43	2.0×10^{-16}	Klin + Meis-40	−0.251	29.34	9.0×10^{-12}
Amb + Meis-60	−0.475	26.75	2.0×10^{-13}	Klin + Meis-60	−0.150	20.74	5.0×10^{-11}
Amb + Meis-80	−0.325	35.12	1.0×10^{-10}	Klin + Meis-80	−0.098	26.69	4.2×10^{-9}
	$R^2 = 0.9956$		$R^2 = 1$		$R^2 = 0.9669$		$R^2 = 0.9212$
	Total AARD	31.10%			Total AARD	26.69%	
	$P \geq 200$	6.15%			$P \geq 200$	6.02%	
Constantinou-40	−0.465	30.06	1.6×10^{-14}	Lyd + Meis-40	−0.389	28.81	5.0×10^{-13}
Constantinou-60	−0.301	22.40	2.0×10^{-11}	Lyd + Meis-60	−0.272	17.79	1.0×10^{-10}
Constantinou-80	−0.188	30.60	1.0×10^{-9}	Lyd + Meis-80	−0.164	29.01	6.0×10^{-9}
	$R^2 = 0.9888$		$R^2 = 0.9827$		$R^2 = 0.9995$		$R^2 = 0.9985$
	Total AARD	27.69%			Total AARD	25.20%	
	$P \geq 200$	6.73%			$P \geq 200$	5.45%	
Joback-40	−0.215	31.18	7.9×10^{-16}	Som + Meis-40	−0.219	27.41	2.5×10^{-11}
Joback-60	−0.084	24.06	2.0×10^{-12}	Som + Meis-60	−0.173	19.66	6.3×10^{-10}
Joback-80	−0.003	33.98	2.5×10^{-10}	Som + Meis-80	−0.057	25.56	3.1×10^{-8}
	$R^2 = 0.9818$		$R^2 = 0.9899$		$R^2 = 0.9414$		$R^2 = 0.9921$
	Total AARD	29.74%			Total AARD	24.21%	
	$P \geq 200$	6.32%			$P \geq 200$	5.94%	

Table 3
Results of the modelling of the Disperse Blue 14/CO_2 phase equilibrium with the three EOS and the VDW MR for two GCM

Joback (T_c = 1137.62 K; P_c = 27.18 bar)			Lyd + Meis (T_c = 790.02 K; P_c = 24.60 bar)		
k_{12}	AARD	P_2^{sat}	K_{12}	AARD	P_2^{sat}
RK			RK		
−0.215	31.18	7.9×10^{-16}	−0.389	28.81	5.0×10^{-13}
−0.084	24.06	2.0×10^{-12}	−0.272	17.79	1.0×10^{-10}
−0.003	33.98	2.5×10^{-10}	−0.164	29.01	6.0×10^{-9}
$R^2 = 0.9818$		$R^2 = 0.9899$	$R^2 = 0.9995$		$R^2 = 0.9985$
Total AARD	29.74%		Total AARD	25.20%	
$P \geq 200$	6.32%		$P \geq 200$	5.45%	
SRK			SRK		
0.178	31.18	2.3×10^{-15}	0.015	29.37	7.8×10^{-13}
0.278	25.27	9.6×10^{-12}	0.133	21.23	5.6×10^{-10}
0.341	34.45	1.0×10^{-9}	0.200	28.67	2.7×10^{-8}
$R^2 = 0.9831$		$R^2 = 0.9838$	$R^2 = 0.9753$		$R^2 = 0.9871$
Total AARD	30.30%		Total AARD	26.42%	
$P \geq 200$	6.25%		$P \geq 200$	6.41%	
PR			PR		
−0.102	30.37	6.3×10^{-15}	−0.312	28.31	1.6×10^{-12}
0.093	24.37	4.0×10^{-11}	−0.122	19.99	7.9×10^{-10}
0.225	29.46	7.8×10^{-9}	−0.015	27.48	3.1×10^{-8}
$R^2 = 0.9878$		$R^2 = 0.9885$	$R^2 = 0.9746$		$R^2 = 0.9872$
Total AARD	28.07%		Total AARD	25.26%	
$P \geq 200$	6.54%		$P \geq 200$	5.11%	

4. Results and discussion

4.1. Estimated properties

The critical properties of Disperse Blue 14 obtained using combinations of GCM are shown in Table 1. These particular GCM were chosen because they are reported in the literature to be the most useful.

Four GCM depend on T_b to calculate T_c but cannot estimate this value (Ambrose, Klincewicz–Reid, Lydersen and Somayajulu); these GCM were combined with the GCM developed by Meissner. The Joback GCM, in which T_c depends on T_b but also estimates the value of the latter, and the GCM of Constantinou–Gani, which estimates both parameters independently, are the only two methods that were used without combination with another GCM.

The GCM that allows T_c to be estimated without requiring T_b, i.e. the Constantinou–Gani method, gives rise to a very similar T_c value to that estimated with the GCM of Ambrose, Lydersen and Somayajulu, when the T_b value is estimated with the Meissner GCM. The Joback GCM estimates the highest critical temperature value. This situation was also found for the other two solutes studied [37,53]. All of the estimated P_c values are in the range of 20–27 bar.

4.2. Correlation results

Given the large number of results generated in this study, only the most important conclusions will be discussed. The results obtained with the RK EOS and VDW MR with each of the GCM are shown in Table 2. These data elucidate the influence of the estimation method for parameters required for thermodynamic modelling.

The R^2 values resulting from the adjustment of P_2^{sat} to the Clapeyron equation and also the lineal adjustment of k_{12} with the temperature are also shown.

The calculated solubility data did not fit appropriately for pressures of 100 and 150 bar in any of the cases investigated. However, at pressures above 150 bar, the agreement between calculated and experimental data can be considered very good in all cases. For the three EOS, when the methods shown in Table 2 were used, the AARD values obtained are in the range 25–30%.

As can be observed in Table 2, the use of the RK EOS gives AARD values of around 6% in all the cases where the pressure is above 150 bar. If k_{12} values are considered, in most cases values of R^2 around 0.99 are obtained when k_{12} is adjusted lineally with T.

In an effort to study easily the influence of the GCM and the EOS, two GCM with different values of T_c and P_c were chosen. The results for the three EOS are shown in Table 3 for each of these methods.

Table 4
Relationship between k_{12} and T

EOS	Joback	Lyd + Meis
RK	$k_{12} = 0.0053T - 1.8664$	$k_{12} = 0.0056T - 2.1490$
SRK	$k_{12} = 0.0041T - 1.0190$	$k_{12} = 0.0046T - 1.4258$
PR	$k_{12} = 0.0082T - 2.6515$	$k_{12} = 0.0074T - 2.6233$

If the cases of Joback and Lyd + Meis are analysed for the three EOS one can draw the following conclusions. Differences in the values of AARD, k_{12} and P_2^{sat} exist regardless of the GCM used. For a given GCM, the AARD values are reasonably similar on using either of the three EOS.

Significant differences in the values of P_2^{sat} are not observed regardless of the EOS used. However, as can be observed in Table 4, the relationship between k_{12} and T depends on the EOS used more than on the GCM chosen.

For most of the GCM, the best adjustments in k_{12} with T and of P_2^{sat} to the Clapeyron equation are obtained when the RK EOS is used. However, modelling of the Disperse Blue 14/CO_2 equilibrium can be performed satisfactorily using any of the three EOS and using any of the GCM studied in this work.

By way of summary, experimental solubility data for Disperse Blue 14 together with those calculated with the RK EOS and the Lyd + Meis GCM are shown in Fig. 2. Experimental solubility data for Disperse Blue 14 together with those calculated with the SRK EOS and the same GCM are shown in Fig. 3 and the corresponding case with the PR EOS in Fig. 4.

5. Conclusions

The Redlich–Kwong, Soave–Redlich–Kwong and Peng–Robinson equations of state provide good

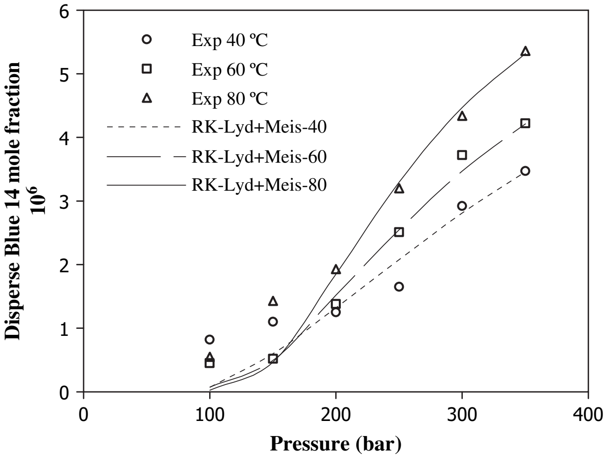

Fig. 2. Solubility of Disperse Blue 14 in supercritical carbon dioxide: experimental results and results obtained by thermodynamic model with RK EOS and Lyd + Meis GCM.

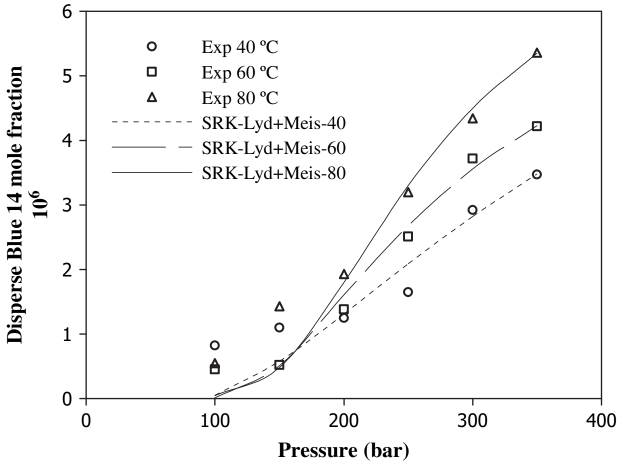

Fig. 3. Solubility of Disperse Blue 14 in supercritical carbon dioxide: experimental results and results obtained by thermodynamic modelling with SRK EOS and Lyd + Meis GCM.

predictions for the solid–fluid equilibrium of the Disperse Blue 14/CO_2 system. Significant differences were not observed in the values of AARD, P_2^{sat} and the trends obtained with each EOS used in this work when a given GCM was chosen. More significant differences are, however, observed in the values of AARD and the solid sublimation pressure when a different GCM is used. In all cases, the parameter k_{12} increases lineally with temperature and the relationship between k_{12} and T depends on the EOS used. The solute sublimation pressure is adjusted correctly to the Clapeyron equation.

The results obtained in predicting the solubility show that the choice of GCM has a greater influence than the choice of one of the three equations of state investigated.

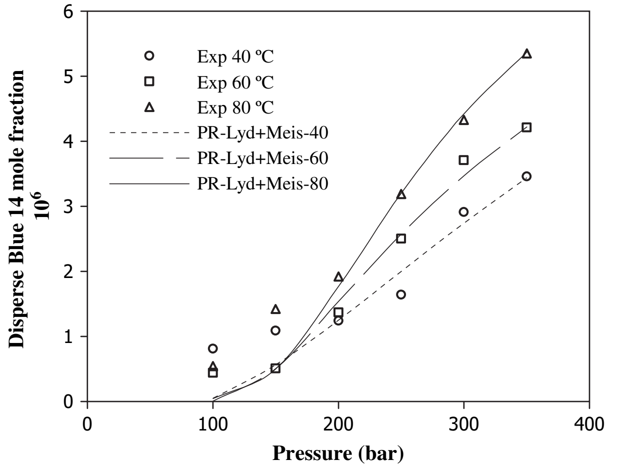

Fig. 4. Solubility of Disperse Blue 14 in supercritical carbon dioxide: experimental results and results obtained by thermodynamic modelling with PR EOS and Lyd + Meis GCM.

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