Data Article

Data solubility and parameters of adjustments ($\alpha$ and $\beta$) of phenanthrene in supercritical CO$_2$ employing the modified Redlich–Kwong equation

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ABSTRACT

This article contains data related to the research article entitled “Calculation method for determining Phenanthrene solubility in supercritical CO$_2$ employing Redlich–Kwong modified equation” (Colpas et al., 2018) [1]. The presented data gives information on the physical properties of the solute and the solvent. The experimental solubilities of phenanthrene in equilibrium and those calculated using the modified Redlich–Kwong equation with the inclusion of the adjustment parameters $\alpha$ and $\beta$ are shown, see Colpas et al. (2018) [1] and “Modified Redlich–Kwong equation of state for supercritical carbon dioxide” (Heidaryan and Jarrahian, 2013) [7]. The mean squared error (MSE) was calculated for the supercritical Phenanthrene–CO$_2$ system at different temperatures above the critical point of the solvent.

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Specifications table

| Subject area            | Chemical Engineering                  |
|-------------------------|---------------------------------------|
| More specific subject area | Thermodynamics/Equilibrium of solids in supercritical fluids |
| Type of data            | Tables                                |
| How data was acquired   | Employing the modified Redlich–Kwong equation, the non-linear simplex method to optimize the values, published literature. |
| Data format             | Raw and Analyzed                      |
| Experimental factors    | Phenanthrene’s solubilities in supercritical CO₂ was calculated using the modified Redlich–Kwong equation including adjustable parameters such as alpha and beta (α and β). A comparison of the experimental data was made through an objective function optimizing alpha and beta values employing a simplex non-linear method. |
| Experimental features   | Published data is used to calculate the solubilities of phenanthrene extracted with carbon dioxide under supercritical conditions at different temperature values. |
| Data source location    | Universidad de Puerto Rico. Mayaguez. Puerto Rico. |
| Data accessibility      | Data are available in this article    |
| Related research article| Colpas, C.A., Tarón, D.A., and González, C.R. Calculation method for determining phenanthrene solubility in supercritical CO₂ employing Redlich–Kwong modified equation. Contemporary Engineering Sciences. 11 (40) (2018): 1971–1981. [1] |

Value of the data

- The calculated solubility data are useful for comparisons with those obtained using modified state equations with different adjustment parameters.
- The α and β parameters avoid the use of critical conditions of the solute, making relevant the solubility data calculated to apply to systems where the solute is a thermolabile substance.
- The average quadratic error (EQA) data indicate that the calculation method applies to other systems of interest for the pharmaceutical, food and chemical industry mainly.

1. Data

The data presented in this article include the experimental solubility of Phenanthrene (Y) at different temperatures and pressures in carbon dioxide under supercritical conditions [2]. Table 1. The physical properties of the solvent; molecular weight (M), critical pressure (Pc), critical temperature (Tc), acentric factor (ω), Table 2. The properties of the solute; molecular weight (M), A and B (variables in Redlich–Kwong equation of state) and molar volume (V̅mol), they were obtained from the literature [3–5]. The solubility values calculated using the modified Redlich–Kwong equation of state with adjustable parameters (α and β) are shown in Table 3.

2. Experimental design, materials and methods

The solubility data are determined by employing the modified Redlich–Kwong equation of state. The modification of the equation was made from the inclusion of adjustable parameters called alpha and beta (α and β), which are relevant because when they are used it is not necessary to know the
Table 1
Experimental data of solubility in equilibrium of Phenanthrene in supercritical CO₂.

| T = 318 K | P₂ (MPa) | Y Molar fraction | T = 328 K | P₂ (MPa) | Y Molar fraction | T = 338 K | P₂ (MPa) | Y Molar fraction |
|-----------|---------|-----------------|-----------|---------|-----------------|-----------|---------|-----------------|
| 12        | 8.49 × 10⁻⁴ |                | 12        | 4.65 × 10⁻⁴ |                | 12        | 3.28 × 10⁻⁴ |                |
| 16        | 11.4³ × 10⁻³ |                | 16        | 1.51 × 10⁻³ |                | 16        | 1.18 × 10⁻³ |                |
| 20        | 1.70 × 10⁻³ |                | 20        | 2.14 × 10⁻³ |                | 20        | 2.37 × 10⁻³ |                |
| 24        | 2.23 × 10⁻³ |                | 24        | 2.79 × 10⁻³ |                | 24        | 3.28 × 10⁻³ |                |
| 28        | 2.28 × 10⁻³ |                | 28        | 3.19 × 10⁻³ |                | 28        | 3.84 × 10⁻³ |                |

Table 2
Physical properties of the solute.

| Solute       | M (g/mol) | Pₑ (MPa) | Tₑ (K) | ω | A | B (k) | 10⁻³ × V⁰ (M³/mol) | Refs. |
|--------------|-----------|----------|--------|---|---|-------|-------------------|-------|
| Phenanthrene | 178.24    | 3.17     | 882.55 | 0.3299 | 14.631 | 4873.4 | 0.1512 | [3–6] |

*Pₑ, Tₑ and ω from Refs. [3,6]; A and B from Refs. [4,6]; V⁰ from Refs. [5,6].

solute critical conditions. The solubilities values (calculated and experimental) are compared by an objective function which is optimized by applying the non-linear simplex method.

2.1. Mathematical details

The basic equation used to calculate the solubility of solids with low vapor pressure in supercritical fluids can be expressed as:

\[ y_2 = \frac{p^{\text{sat}}_2}{P_2} \exp \left( \frac{V^{\text{sol}}_2 p}{RT} \right) \]  

where \( y_2 \) is the solubility of solids with low vapor pressure in supercritical fluids, the fugacity coefficient, \( p^{\text{sat}}_2 \) the saturation pressure, \( V^{\text{sol}}_2 \) is the solid molar volume of the solute, \( R \) the universal constant of the gases, \( T \) the temperature and \( P \) the system pressure. Subscript 2 refers to the solid component. All terms can be obtained experimentally except \( \phi^V_2 \). The Redlich–Kwong equation is used to calculate the fugacity coefficient, the expression for the calculation is as follows:

\[ \ln \phi^V_2 = (Z - 1) b_2 b_1 - \ln(Z - B) - \frac{a}{b} b_1 \left[ \frac{2(y_1 a_1 y_2 a_2)}{a} - 1 \right] \ln \frac{Z + B}{Z} \]  

where \( A \) and \( B \) are the adjustable parameters, \( a_1 \) and \( b_1 \) are the solute Van der Waals parameters of solute, \( a_2 \) and \( b_2 \) are the solvent Van der Waals parameters, \( a \) and \( b \) are the mixture parameters and \( Z \) is the compressibility factor, which depend on the solubility. For the fluid phase, \( a \) and \( b \) were calculated employing Van der Waals mixing rule, it can be observed that solubility is a \( Z \) function.

To infinite dilution la Eq. (2) can be rewritten as follows:

\[ \ln \phi^\infty_2 = (Z - 1) b_2 b_1 - \ln(Z - B) - \frac{A}{B} \left( \frac{a_2}{a_1} - \frac{b_2}{b_1} \right) \ln \frac{Z + B}{Z} \]  

The final equation for the fugacity coefficient at infinite dilution is:

\[ \ln \phi^\infty_2 = \beta(Z - 1) - \ln(Z - B) + \frac{A}{B} (\beta - 2\alpha) \ln \frac{Z + B}{Z} \]  

where \( \alpha \) is the adjustment parameter with respect to the molecular interactions between the solute and the solvent, \( \beta \) the adjustment parameter in relation to the molecular size between the solute and the solvent.
Table 3
Solubility data calculated for the supercritical phenanthrene-CO₂ system using the modified Redlich–Kwong equation of state.

| Supercritical temperature (K) | 
|-----------------------------|
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The mean squared error was calculated through the following equation

\[
ECM = 100 \sqrt{\frac{1}{N_p} \sum_{i=1}^{N_p} \left( y_{i,\text{cal}} - y_{i,\text{exp}} \right)^2}
\]  

(5)

where \( y_{i,\text{cal}} \) is the solubility calculated from component \( i \), \( y_{i,\text{exp}} \) the experimental solubility of component \( i \) and \( N_p \) is the data number.

The reader can find further details in our previous paper [1], and another manuscript [2].

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Transparency document. Supplementary material

Transparency data associated with this article can be found in the online version at https://doi.org/10.1016/j.dib.2018.10.038.
References

[1] C.A. Colpas, D.A. Tarón, C.R. González, Calculation method for determining phenantrene solubility in supercritical CO₂ employing Redlich–Kwong modified equation, Contemp. Eng. Sci. 11 (40) (2018) 1971–1981.
[2] C.A. Caballero, N.L. Hernández, L.A. Estevéz, Calculation of interaction parameters for binary solid-SCF equilibria using several EOS and mixing rules, J. Supercrit. Fluids 5 (4) (1992) 283–295.
[3] E. Kosal, G.D. Holder, Solubility of anthracene and phenantrene mixtures in supercritical carbon dioxide, J. Chem. Eng. Data 32 (1987) 148.
[4] K.P. Johnston, D.H. Ziger, C.A. Eckert, Solubilities of hydrocarbon solids in supercritical fluids. The augmented Van der Waals treatment, Ind. Eng. Chem. Fundam. 21 (1982) 191.
[5] J.A. Dean, Lange's Handbook of Chemistry, 13th ed., McGraw-Hill, New York, 1987.
[6] T.R. Kumik, J.S. Holla, C.R. Reid, Solubility of solids in supercritical carbon dioxide and ethylene, J. Chem. Eng. Data 26 (1) (1981) 47–51.
[7] E. Heidaryan, A. Jarrahiyan, Modified Redlich–Kwong equation of state for supercritical carbon dioxide, J. Supercrit. Fluids 81 (2013) 92–98.