INFLUENCE OF PROPERTY ESTIMATION TECHNIQUES ON THERMODYNAMIC MODELING OF SOLUBILITY OF C. I. DISPERSE ORANGE 30 DYE IN SUPERCRITICAL CO$_2$

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ABSTRACT

The present work deals with the study of thermodynamic modeling of solubility of C. I. disperse orange 30 (O30) dye in supercritical CO$_2$ using Peng-Robenson equation of state (PR-EOS). The sensitivity of critical properties in the calculations was also studied.

The results of model showed good agreement with the experimental data of the system taken and the study proved that the choice of the technique to calculate thermodynamic properties is very important for obtaining good results in the phase equilibrium calculations.

Keywords: Phase behavior, C. I. disperses orange 30 dye, critical properties estimation techniques, CO$_2$, PR-EOS.

NOTATIONS

$A_1$, $A_2$, $A_3$, and $A_4$  constants in equation (18).  
$A$, $B$  modified adjusting parameters in equation of state of mixture.  
$a_i$, $b_i$  parameters in equation of state of pure component.  
$a_m$, $b_m$  parameters in equation of state of mixture .  
$f_i^{SCF}$  fugacity in fluid phase, bar.  
$f_i^s$  fugacity in solid phase, bar.
$k_{ij}$ interaction parameter in mixing rules, equation (9).
$M_w$ molecular weight.
$n$ number of moles.
$n_c$ number of carbon atoms.
$N$ number of data points.
$P$ total system pressure, bar.
$P_c$ critical pressure, bar.
$P_{sub}$ sublimation pressure, bar.
$R$ universal gas constant ($0.08314\ \text{bar m}^3/\text{Kmol K}$).
$T$ absolute temperature, K.
$T_b$ normal boiling point, K.
$T_c$ absolute critical temperature, K.
$T_r$ reduced temperature ($T/T_c$).
$v_i^s$ molar volume of pure solid, (lit. / mol).
$V$ total system volume, (lit.).
$v^v$ molar volume of vapor phase, (lit./mol).
$y_{calc}$ calculated or predicted mole fraction solubility.
$y_{exp}$ experimental mole fraction solubility.
$y_i$ mole fraction solubility of component i.
$Z$ compressibility factor.

Greek letters
$\alpha$ quantity estimated in equation (30).
$\beta$ quantity estimated in equation (31).
$\theta$ reduced normal boiling temperature ($T_b/T_c$).
$\omega$ acentric factor.
$\phi^v_i$ fugacity coefficient of component i in vapor phase.
$\kappa$ quantity estimated in equation (4).
$\phi^{SCF}_i$ gas phase fugacity coefficient, equation (11).

Superscripts
$SCF$ supercritical fluid.
$S$ solid.
$Sub$ sublimation.
$v$ vapor.

Subscripts
$c$ critical property.
$m$ mixture.
$r$ reduce property.
$ij$ component indices.
exp  experimental measurement.
calc  predicted value.

Abbreviations
AARD  absolute average relative deviation.
C. I.  Color Index.
EOS  equation of state.
O30  C. I. disperses orange 30 dye.
PR  Peng-Robinson.
SCF  Supercritical Fluid.
SRK  Soave –Redlich- Kwong

INTRODUCTION
The conventional wet-dyeing industry, which discharges considerable amounts of wastewater containing highly concentrated, very little biodegradable surfactants, has been continuously raising pollution problems worldwide. Supercritical fluid dyeing process is environmentally friendly because it does not require any surfactant or dispersing agent\(^1,2\). Furthermore, energy consumption may be only a half that of the conventional dyeing process as the drying step is not necessary in the supercritical fluid dyeing.

Although there has been much research on solid solubility in supercritical fluid (SCF), the phase behavior of solids with very high molecular weights has not been fully understood yet. Some empirical equations have been used to correlate the solubility of large molecular-weight solids with pressure or density of the fluid\(^3\).

Abdul Mun’em\(^4\) measured the solubility of solid components in supercritical CO\(_2\) at temperature range (308.15 – 323.15) K and pressure range (80 – 200) bar and the experimental data are correlated with three cubic equations of state which are Redlich-Kwonge (RK), Soave-Redlich-Kwonge (SRK) and PR. Serwan\(^5\) studied the phase equilibria modeling for separation of solid mixtures by supercritical CO\(_2\) on Excel program using PR-EOS.

Hartono et al.\(^6\) used six different cubic equations of state to predict the solubility of solids and they shown that the two-parameters Mohsen-Nia-Moddaress-Mansoori (MMM) equation is more accurate than five of the other equations. Beak et al.\(^7\) measured and correlated the solubility of C. I. disperse orange 30 dye (O30) in CO\(_2\) at temperatures between 313 and 393 K and at pressures between 110 and 330 bar.
Phase equilibrium calculation using a thermodynamic model requires thermodynamic properties that were not found in the literature and must therefore be predicted. These properties are critical temperature, critical pressure, the acentric factor, and the parameters presented in the equation that calculated the saturation pressure of the compound. Therefore, different property estimation techniques are investigated in present work and their influence on the ability to correlate the experimental solubility data obtained from literatures (7) of C. I. disperse orange 30 dye (Fig. 1) as a solid component in supercritical CO\textsubscript{2} using PR-EOS.

![Molecular structure of C. I. Disperse Orange 30 dye](image)

Fig. (1). The molecular structure of C. I. Disperse Orange 30 dye (7).

**THERMODYNAMIC MODELING**

Although solubility measurements in supercritical CO\textsubscript{2} are the first key step in evaluating the viability of supercritical fluid processes, thermodynamic modeling can provide feasibility analysis and reduce the number of experimental measurements required (8). On the other hand, it is important to note that rigorous thermodynamic modeling of solubilities of compounds of high molecular weight interest can be difficult due to an almost complete lack of knowledge of the physical properties necessary for pure molecule parameter used in equation of state.

The PR-EOS was chosen to model the high-pressure phase behavior with quadratic Van der Waals mixing rules and take the following form (9):

\[
P = \frac{RT}{(\varphi - b)} - \frac{a}{[\varphi(\varphi + b) + b(\varphi - b)]} \quad \ldots (1)
\]

where,

\[
a = a(T_\varphi)\kappa(T,\omega) \quad \ldots (2)
\]

\[
\kappa(T,\omega) = [1 + \kappa(1 - T^{0.5})]^2 \quad \ldots (3)
\]

\[
\kappa = 0.37464 + 1.54226\omega - 0.26992\omega^2 \quad \ldots (4)
\]
In general an equation of state is developed first for pure component, and then extended to mixtures through the use of mixing rules for combining the pure component parameters. For the mixture, the conventional Van der Waals mixing rules were used:

\[
a_m = \sum_i \sum_j y_i y_j a_{ij} \quad \ldots \quad (7)
\]

\[
b_m = \sum_i y_i b_i \quad \ldots \quad (8)
\]

where,

\[
a_{ij} = (a_i a_j)^{0.5} (1 - k_{ij}) \quad \ldots \quad (9)
\]

where \(a_i\) and \(b_i\) are calculated from equations (2) and (6) using the critical pressure \(P_c\), critical temperature \(T_c\) andacentric factor \(\omega\) for each component. In equation (9), \(k_{ij}\) is the binary interaction parameter, which has a non-zero value and for an \(n\)-component mixture there are \(\frac{n(n-1)}{2}\) possible binary interaction parameters.

**Solid - Fluid Phase Equilibrium**

The most important application of the equation of state approach lies in computing solubilities of relatively nonvolatile solids in supercritical fluids. To analyze this phenomenon, it will start with the equality of the species fugacities in each phase. However, since the fluid (liquid, gas, or supercritical fluid) is not present in the solid (or it contains a negligible amount), two simplifications arise. First, the equilibrium criterion applies only to the solid solute, which is denoted by the subscript \(i\), and second; the solid phase fugacity of the solute is that of the pure solid. Thus a single equilibrium relation will be presented as \((10, 11)\):

\[
f_i^S(T, P) = f_i^{SCF}(T, P, y_i) \quad \ldots \quad (10)
\]

where the superscript \(S\) and \(SCF\) refer to the pure solid and supercritical fluid phases, respectively, then \(f_i^{SCF}\) can be expressed as:

\[
f_i^{SCF} = \phi_i^{SCF} y_i P \quad \ldots \quad (11)
\]
where \((y_i)\) is the mole fraction of solid in the gas phase, \(\phi_i^{SCF}\) is the gas phase fugacity coefficient, \(f_i^{s}\) is the fugacity of solid and it has pressure units.

For each component \((i)\) in the fluid phase (vapor, liquid phase or supercritical state)\(^{(12)}\):

\[
\ln \phi_i = \frac{1}{RT} \int \left[ \left( \frac{\partial P}{\partial n_i} \right)_{T, V, n_j} - \frac{RT}{V} \right] dV - \ln Z
\]

\[
\text{......} (12)
\]

where \(V\) is the total system volume, \(n_i\) and \(n_j\) are the number of moles of components \(i\) and \(j\) respectively.

When the PR-EOS is introduced into Eq. (12) using mixing rules given by Eq. (7) and (8), the following closed-form expression for fugacity coefficient is obtained and used in all phases,

\[
\ln \phi_i = \frac{b_i}{b_m}(Z-1) - \ln(Z-B) + \frac{A}{2\sqrt{2B}} \left[ \frac{b_i}{b_m} - \frac{2\sum y_j d_j}{\alpha_m} \right] \ln \left( \frac{Z+2414B}{Z-0.414B} \right)
\]

\[
\text{......} (13)
\]

and when replacing \(v\) in Eq. (1) in term of \(ZRT/P\), gives the cubic equation of PR-EOS as:

\[
Z^3 - (1-B)Z^2 + \left( A - 2B - 3B^2 \right)Z - \left( AB - B^2 - B^3 \right) = 0
\]

\[
\text{......} (14)
\]

where \(Z\) is compressibility factor and, \(A\) and \(B\) are defined as,

\[
A = \frac{a_n P}{(RT)^2}
\]

\[
\text{......} (14a)
\]

\[
B = \frac{b_m P}{RT}
\]

\[
\text{......} (14b)
\]

Because the solid phase is normally considered a pure solid (i.e. the SCF solvent does not dissolve in the solid), the fugacity \(f_i^{s}\) is

\[
f_i^{s} = P_i^{sub}(T)\phi_i^{sub}(T,P_i^{sub})\exp \left[ \int_{P_i^{sub}}^{P} \left( \frac{D_i^s}{RT} \right) dP \right]
\]

\[
\text{......} (15)
\]

where \(P_i^{sub}(T)\) is the sublimation or vapor pressure of the pure solid at the system temperature, \(v_i^{s}\) the molar volume of the pure solid and is independent of pressure, \(\phi_i^{sub}(T,P_i^{sub})\) is the fugacity coefficient at \(T\) and \(P_i^{sub}\) to be assumed unity, and the exponential term is the Poynting factor correction for the fugacity of the pure solid. Therefore,
combining Eqs (11) and (15), the mole fraction solubility of a heavy nonvolatile solid in the SCF solvent phase now becomes,

$$y_i = \frac{P_i^{sub}(T) \exp \left( \frac{v_i' (P - P_i^{sub})}{RT} \right)}{\phi_i^{SCF} p}$$ .... (16)

The partial molar volume of the solid components at all pressures and temperatures is assumed equal to its molar volume at atmospheric pressure and 298K, and this will be closer to the truth\(^{(13)}\).

**ESTIMATION OF PROPERTIES**

To calculate the solubility and phase stability of a solute in a supercritical fluid it is necessary to have critical properties andacentric factors of all components, and molar volumes and sublimation pressures of the solid components. When some of these values are not available, as is the case here, estimation techniques must be employed. When neither critical properties noracentric factors are available in the literature, it is desirable to have the normal boiling point \(T_b\) of the compound since some estimation techniques require only \(T_b\) and molecular structure. Also, vaporization, sublimation and/or fusion curves and normal melting point information might be of help for the estimation of \(T_b\). Some of the estimation techniques used below, where only the molecular structure and/or molecular weight are required.

In the following subsections, different property estimation techniques used in this work will be discussed. The estimated \(T_c\), \(P_c\) and \(\omega\) as parameters used in the Peng-Robinson EOS; beyond that we do not assign any physical significance to the values obtained. C. I. disperse orange 30 dye is a typical solute of high molecular mass for which critical constants are not available in the literature.

The properties found in the literature or estimated with the methods explained below are summarized in Table (1). Note that with the objective of obtaining the best fit of the solubility behavior of C. I. disperse orange 30 dye in supercritical CO\(_2\), there are different sets of properties reported depending on the estimation method used.

**Boiling Point**

As mentioned above, the normal boiling point of a component is one of the key properties for the estimation of other parameters or properties. Since there is no experimental boiling point available, two
methods were used to estimate boiling points: the Joback group contribution approach and by simulation with n-alkanes having the same molecular weight using the Tsonopoulos\(^{(14)}\) method of the n-alkanes.

The Joback group contribution approach is used to obtain an approximate estimate of \(T_b\) with the following correlation:

\[
T_b = 198 + \sum \Delta_b, \quad \text{in} [\text{K}] \quad \text{.... (17)}
\]

Here \(\Delta_b\) represents group increments according to structural information. The tabulated group values are presented in Reid et al.\(^{(15)}\).

Tsonopoulos correlated the \(T_b\) (K) of the n-alkanes with the number of carbon atoms (\(n_c\)) using a simple equation of the form,

\[
\ln (A_i - T_b) = A_2 - A_3 n_c + \frac{A_4}{n_c} \quad \text{.... (18)}
\]

where, \(A_1=1071.28\), \(A_2=6.97569\), \(A_3=0.116307\), \(A_4=2/3\)

To obtain the \(T_b\) of n-alkanes as a function of molecular weight (Mw), the \(n_c\) in Eq. (18) should be replaced by the following simple expression,

\[
n_c = \frac{M_w - 2.0158}{14.0268} \quad \text{.... (19)}
\]

---

**Critical Properties**

Critical properties are crucial for an accurate representation of experimental behavior. In this work, five methods were used to estimate these properties: the Fedors, Joback, Ambrose, Lydersen methods described in detail by Reid et al.\(^{(15)}\) and Perry et al.\(^{(16)}\) and Klincewicz method\(^{(17)}\) group contribution approaches. The Fedors method estimates critical temperature, \(T_c\), using group increments (\(\Delta T\)) according to the molecular structure and Eq. (20).

\[
T_i = 535 \log_{10} \left( \sum \Delta T \right) \quad \text{[\text{K}]} \quad \text{.... (20)}
\]

The Joback group contribution approach is useful in estimating \(T_c\) (Eq.21) as a function of \(T_b\) and group increments (\(\Delta T\)) according to the molecular structure. Critical pressure, \(P_c\), is estimated with Eq. (22) as a function of the number of atoms in the molecule (\(n_A\)) and group increments (\(\Delta P\)). Tabulated values used in this work were obtained from Reid et al.\(^{(15)}\).

\[
T_c = T_b \left[ 0.584 + 0.965 \sum \Delta T - \left( \sum \Delta T \right)^2 \right], \quad \text{[\text{K}]} \quad \text{.... (21)}
\]
\( P_c = \left( 0.113 + 0.0032 n_A - \sum \Delta P \right)^2, \quad P_c [\text{bar}] \quad \ldots \ldots \ldots (22) \)

The Ambrose method is another group contribution approach to estimate the critical temperature and pressure. The method is similar to the previous one, except that the critical pressure is a function of the molecular weight, \( M_w \), of the molecule (Eqs. 23-24).

\[
T_c = T_b \left[ 1 + (1.242 + \sum \Delta T)^{-1} \right], \quad T_c, T_b = \text{[K]} \quad \ldots \ldots (23)
\]

\[
P_c = M_w(0.330 + \sum \Delta P)^2, \quad P_c = \text{[bar]} \quad \ldots \ldots (24)
\]

The Lydersen method is group contribution approach to estimate the critical temperature and pressure and is similar to Ambrose method and the relations are,

\[
T_c = T_b \left[ 0.567 + \sum \Delta T - \left( \sum \Delta T \right)^{\frac{1}{2}} \right], \quad T_c, T_b = \text{[K]} \quad \ldots \ldots (25)
\]

\[
P_c = M_w(0.34 + \sum \Delta P)^2, \quad P_c = \text{[bar]} \quad \ldots \ldots (26)
\]

Klincewicz has refitted correlations for estimating the critical properties of pure components as follow,

\[
T_c = 45.40 - 0.77 M_w + 1.55 T_b + \sum \Delta T, \quad T_c, T_b = \text{[K]} \quad \ldots \ldots (27)
\]

\[
P_c = \left( 0.335 + 0.01 M_w + \sum \Delta P \right)^{\frac{1}{2}}, \quad P_c = \text{[bar]} \quad \ldots \ldots (28)
\]

All methods mentioned above were used with the objective of finding the best fit for the experimental data.

**Acentric factor**

Acentric factor, \( \omega \), for molecule was estimated using the Lee-Kesler correlation Eqs. (29-31), where \( \theta = T_b / T_c \) and the correlation is described in Reid et al. (15).

\[
\omega = \frac{\alpha}{\beta} \quad \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldotted{21}
\]

\[
\alpha = -\ln P_c - 5.972146.0964 \theta^{3/2} + 1.2886 \theta - 0.16934 \theta^2, \quad P_c = \text{[atm]} \quad \ldots \ldots (30)
\]

\[
\beta = 15.2518 - 15.6875 \theta^{-1} - 13.472 \ln \theta + 0.43577 \theta^6 \quad \ldots \ldots (31)
\]

**Sublimation pressure**

The vapor pressures of solid component (C. I. disperse orange 30 dye) studied calculated by the following equation:

\[
\ln(P_{sub}) = 38.3625 - \frac{14613.55}{T} \quad \ldots \ldots (32)
\]
where $P_{\text{sub}}$ in N/m$^2$, $T$ in K and Eq. (32) is obtained by least square fittings method for the experimental values of vapor pressure at different temperatures that exist in literature\(^{(7)}\) and its melting point, 398.56K, and the heat of fusion, 17.08 kJ/mol, were measured by differential scanning calorimeter\(^{(7)}\).

**Molar volume**

Molar volume ($v_i^s$) of the C. I. disperse orange 30 dye is found in literature and its value equal to 273 cm$^3$/mole\(^{(7)}\).

**$k_{ij}$ interaction parameters**

The interaction parameters between the C. I. disperse orange 30 dyes and carbon dioxide at each temperature was obtained by regression of the experimental data and the values are shown in Table (2). The objective function used was the average absolute relative deviation (%AARD), as shown in Eq. (33). Here $y_{i}^{\text{exp}}$ are the experimental data, $y_{i}^{\text{calc}}$ are the predicted values and $N$ is the total number of data points.

$$\%\text{AARD} = \frac{100}{N} \sum_{i=1}^{N} \left| \frac{y_{i}^{\text{exp}} - y_{i}^{\text{calc}}}{y_{i}^{\text{exp}}} \right|$$

............... (33)

**RESULTS AND DISCUSSION**

The critical properties and acentric factor of the C. I. disperse orange 30 dye were predicted using most of the group contribution methods, Joback, Lydersen, Ambrose, Klincewicz, and Fedors when using the normal boiling point ($T_b$) determined by Joback method (Eq. 17) and by simulation with normal alkanes having the same molecular weight (Eq. 18) to study the sensitivity of these properties in the solubility calculations.

The $k_{ij}$ parameters was estimated from combination of the experimental solubility data for C. I. disperse orange 30 dye were collected at 313.15, 333.15, 363.15, and 393.15K and from 110 bar to 330 bar\(^{(7)}\). The values of $k_{ij}$ were increased with temperature increased for all sets (see Table 2). The %AARD values are very sensitive to critical properties of the component studied and the optimum value of it when using set 7.
A comparison between the experimental and calculated solubilities of C. I. disperse orange 30 dye in supercritical CO$_2$ when using set 7 is shown in Fig.s (2-5).

The properties obtained from the Ambrose group (set 7) gave better results than the others and linear relation obtained when regressed the values of $k_{ij}$ and temperatures and taken the following form when using set (7),

$$k_{ij} = [-6.74 + 11.52T(K)] \times 10^{-4}$$

with correlation coefficient and standard error are 0.9995 and 0.00753 respectively. Equation (34) can be used to obtain the value of $k_{ij}$ at other temperatures which is used in the calculations of the solubility of C. I. disperse orange 30 dye in supercritical CO$_2$ by using the purposed thermodynamic model with PR-EOS as shown in Fig.(6) at temperatures 305.15, 353.15, and 373.15K.

**CONCLUSIONS**

The results of model showed good agreement with the experimental data of the system taken and the %AARD ranges from 8.9% to 15.8% when using set 7.

Also, the present work showed that the choice of a group contribution method and the suitable normal boiling point determination is very important to obtain good results in phase equilibrium calculations, and before equilibrium conditions are studied, the physicochemical properties must be obtained.

**REFERENCES**


- 80 -


Table (1)

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<th>(T_b) [K]</th>
<th>(T_c) [K]</th>
<th>(P_c) [bar]</th>
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Table (2)
Binary Interaction Parameters with CO\(_2\) and %AARD.

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<th>(T=363.15)K</th>
<th>(T=393.15)K</th>
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Fig. (2). The solubility of O30 dye in supercritical carbon dioxide as a function of pressure at $T=313.15K$. 

Baek et al., 2004

PR EOS (set 7, $k_{ij} = 0.3640$)
Fig.(3). The solubility of O30 dye in supercritical carbon dioxide as a function of pressure at T=333.15K.
Fig.(4). The solubility of O30 dye in supercritical carbon dioxide as a function of pressure at $T=363.15K$. 

Baek et al., 2004

PR-EOS(set 7, $k_ij=0.4112$)
Fig. (5). The solubility of O30 dye in supercritical carbon dioxide as a function of pressure at $T=393.15\text{K}$.
Fig. (6). The solubility of O30 dye in supercritical carbon dioxide as a function of pressure.
تأثير أساليب تغيير الجذور على نموذج الدينامية الحرارية لدواماني الصبغة البرتقالية الصلبة في ثاني أكسيد الكربون فوق الجر.

عبدا الدوري
أستاذ مساعد كلية الهندسة / جامعة دياeliness / بعقوبة / العراق

تناول البحث دراسة نموذج الدينامية الحرارية لدواماني الصبغة البرتقالية (C.I. disperse orange 30 dye) في ثاني أكسيد الكربون فوق الجر باستخدام معالجة بونغ-روبنسون (Peng-Robenson). زيدت دراسة الحساسية لأساليب تغيير الجذور في الحسابات بين النتائج النموذجية وأن هناك توافقًا جيدًا مع البيانات التجريبية للنظام، وقد كان مدى متوسط النسبة المئوية لموافقة 98%.

ودعت الدراسة أن اختيار أساليب تغيير الجذور مهمًا للحصول على نتائج جيدة في حسابات التوازن التوري في الظروف فوق الجر.