SOLUBILITY PREDICTION OF CO_2 IN SEVERAL PHYSICAL LIQUID SOLVENTS USING CHEMCAD AND HYSYS SIMULATORS

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ABSTRACT:- CHEMCAD and HYSYS process simulators were used to analysis the literature experimental data and predict the solubility of CO_2 in three physical solvents (sulfolane, propylene carbonate (PC), and n-methyl-2-pyrrolidone (NMP)) at different temperatures (298.15 , 313.15 , 323.15, and 373.15 K). Two thermodynamic models were used, the first using Peng-Robinson equation of state (PR-EOS) and the second using Soave-Redlich-Kwong equation of state (SRK-EOS). The solubility data of CO_2 in all three physical solvents systems were correlated with CHEMCAD simulator using the SRK model without modification (k_{ij} = 0).The results showed a small deviation (less than 5%), but higher deviation (about 10%) was noticed only for CO_2-NMP system at temperature 373 K. Whereas the results of PR model showed a high deviation (about 20%) with all the three physical solvents systems. Modifications performed by editing user defined binary interaction parameters (BIP) of the systems used, give good results for both simulators.

Keywords:- Solubility prediction of CO_2, Physical solvents, CHEMCAD and HYSYS Process Simulators, PR-EOS, SRK-EOS.

NOMENCLATURE

A, B: modified adjusting parameters in equations of state of mixture.

a_i, b_i : parameters in equations of state of pure component.

a_m, b_m : parameters in equations of state of mixture .

A_{ij}, B_{ij}, C_{ij} : Constants of the binary interaction parameter correlation (eq.23).

f : fugacity, bar

k_{ij} : binary interaction parameter between component i and j.

K: Equilibrium constant.

κ : quantity estimated from equation (10).

n_i : number of moles of component i, mole.

N : number of components.

P: Total pressure, bar.

R : universal gas constant, lit. bar/mole K.

T: absolute temperature, K.

v : total system molar volume , lit./mole.

x, y : liquid and vapor mole fractions, respectively.

x_{CO2}: CO₂ mole fraction in liquid phase.

Z : compressibility factor.

$\hat{\phi}_i^{\lambda}$: Partial liquid fugacity coefficient.

$\hat{\phi}_i^{v}$: Partial vapor fugacity coefficient.

ω : acentric factor.

Subscripts and Superscripts

c : critical condition.

i,j : component.

m : mixture.

r : reduced property.

INTRODUCTION

The investigation of gaseous solutes solubility in liquid is a fundamental importance for design of gas absorption processes to purify industrial and natural gases which frequently contain large quantities of carbon dioxide (CO_2) and hydrogen sulfide (H_2S).Absorption with physical solvents presents the advantage of low energy requirements in the regeneration step.

Furthermore they are often preferred for treating gas streams at high pressure with high concentrations of the acid gases (CO_2 and H_2S) [1] .Some physical solvents such as sulfolane, n-methyl-2-pyrrolidone (NMP) and propylene carbonate (PC) used in the processing of gases which has a strong affinity for acid gases (CO_2 and H_2S) present in many natural and refinery

gas streams. In general, the economics of CO_2 recovery is strongly influenced by the partial pressure of CO_2 in the feed gas. At low partial pressures, physical solvents are impractical because the compression of the gas for physical absorption is expensive. However, if the gas is available at high pressure, physical solvents might be a better choice than chemical solvents. [2].

Kassim et al. [3] measured the solubility of CO_2 in the extraction solvents 1-methyl-2-pyrrolidone, 4-formylmorpholine , γ-butyrolactone , sulfolane , 1,4-dioxane over the temperature range (303.15-333.15) K at a partial pressure of 1 atm using the falling-film flow technique. For all systems, the solubility was found to be decreased with increasing temperature. Agreement with solubilities predicted by the Redlich-Kwong equation of state (RK-EOS) for binary systems was with in $\pm$ 3%.

Murrieta-Guevara et al. [1] measured the solubility of carbon dioxide and hydrogen sulfide in propylene carbonate, n-methylpyrrolidone, sulfolane at several temperatures ranging from 298.15K to 373.15 K and pressure range (0.01-23.30) bar and they correlated the experimental data with Soave-Redlich-Kwong equation of state (SRK-EOS) using binary interaction parameter and they derived the values of Henry's constants and the heat of solution from solubility data.

Roberts and Mather [4] studied the solubility of H_2S and CO_2 in sulfolane and 1-dioxide at 313.15K and 373.15K and pressure up to 23.50 bar and 59 bar respectively. The Henry's constant obtained from the data is in good agreement with those of Rivas and Prausnitz [5]. The fugacity of pure solute gases was calculated using Peng-Robenson equation of state (PR-EOS).

Jou et al. [2] measured the solubility of H_2S, CO_2, CH_4, and C_2H_6 in sulfolane at the temperature range (298.15-403.15)K and pressures up to 78 bar. The experimental data were correlated by the PR-EOS and interaction parameters have been obtained for these systems as a linear and function of temperature.

Henni and Mather [6] measured the solubility of CO_2 in triethylene glycol monomethyl ether (TEGMME) at temperatures 313.15, 343.15, and 373.15K and pressures up to 88 bars.

TEGMME belongs to the same chemical family as the dimethyl ether of tetraethylene glycol (DMETEG), but it costs four times less than the DMETEG eight times less than N-formyl morpholine.

Abdul Mun'em and Arkan [7] were prepared a thermodynamic model for prediction of gas-liquid equilibrium at high pressures and different temperatures for the binary systems of

carbon dioxide (1) with each of the one of the liquid physical solvents (2) (sulfolane, n-methyl-2-pyrrolidone and propylene carbonate) using PR-EOS with different mixing rules to show the effect of the type of mixing rule used.

With the development of computer and computer programs the use of analytical expressions to interpolate, extrapolate and even predict thermodynamic information has become of increasing importance for process design and for modeling of process operation. Therefore the present work was undertaken to verify the suitability of the application of CHEMCAD and HYSYS simulators thermodynamic models in the prediction and correlation of the solubility of CO_2 in a number of physical solvents (sulfolane, propylene carbonate (PC), and n-methyl-2-pyrrolidone (NMP)) at high pressures and different temperatures.

THEORY AND EQUATION OF STATE APPROACH

Vapor-liquid equilibrium (VLE) relationships are needed in the solution of many engineering problems. The required data can be found by experiment, but such measurements are seldom easy, even for binary systems, and they become rapidly more difficult as the number of constituent species increases. This is the incentive for application of thermodynamics to the calculation of phase-equilibrium relationships.

A measure of how a given chemical species distributes itself between liquid and vapor phases is the equilibrium ratio:

$$K_i = \frac{y_i}{x_i} \tag{1}$$

Moreover, it characterizes lightness of a constituent species. For a light species, there are tending to concentrate in the vapor phase, $K > 1$; for a heavy species, tending to concentrate in the liquid phase, $K < 1$ [8]. For equilibrium conditions we have:

$$f_i^{\nu} = f_i^{\lambda} \tag{2}$$

The defining equation for the fugacity coefficient may be applied to each phase:

Vapor phase: $f_i^{\nu} = \phi_i^{\nu} y_i P$ $\tag{3}$

Liquid phase: $f_i^{\lambda} = \phi_i^{\lambda} x_i P$ $\tag{4}$

Then

$$\hat{\phi}_i^{\nu} y_i = \hat{\phi}_i^{\lambda} x_i \tag{5}$$

From Eq. (1) and (5):

$$K_i = \frac{\hat{\phi}_i^{\lambda}}{\hat{\phi}_i^{v}} \tag{6}$$

The most popular equations of state are SRK-EOS and PR-EOS. They normally use three pure-component parameters per substance. Thus, in the present work, SRK-EOS and PR-EOS were chosen to model the high-pressure phase behavior with quadratic van der Waals mixing rules and are take the forms shown in Table (1).

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:

$$a_m = \sum_{i}^{N} \sum_{j}^{N} y_i y_j a_{ij} \tag{13}$$

$$b_m = \sum_{i}^{N} y_i b_i \tag{14}$$

where,

$$a_{ij} = \left(a_i a_j\right)^{0.5}\left(1 - k_{ij}\right) \tag{15}$$

where a_i and b_i are calculated using the critical pressure P_c, critical temperature T_c and acentric factor ω for each component. The interaction parameter, k_{ij} in equation (15) is an adjustable value characterizing the binary formed by component i and j, $k_{ij} = k_{ji}$ and $k_{ii} = 0$.

For each component (i) in the fluid phase (vapor or liquid phase) [9],

$$\ln \hat{\phi}_i = \frac{1}{RT} \int_{\upsilon^v}^{\infty} \left[\left(\frac{\partial P}{\partial n_i}\right)_{T,\upsilon,n_j} - \frac{RT}{\underline{V}}\right] d\underline{V} - \ln Z \tag{16}$$

where $\underline{V}$ is the total system volume, n_i and n_j are the number of moles of components i and j respectively.

When the cubic equation of state (SRK or PR) is introduced into Eq. (8) using mixing rules given by Eqs. (7a) and (7b), the following closed-form expression for fugacity coefficient is obtained and used in all phases,

SRK-EOS:

$$\ln \hat{\phi}_i = \frac{b_i}{b_m}(Z-1) - \ln\left[Z\left(1 - \frac{b_m}{\upsilon}\right)\right] + \frac{a_m}{b_m RT}\left[\frac{b_i}{b_m} - \frac{2\sum_j x_j a_{ji}}{a_m}\right]\ln\left(1 + \frac{b_m}{\upsilon}\right) \tag{17}$$

PR-EOS:

$$\ln \hat{\phi}_i = \frac{b_i}{b_m}(Z-1) - \ln\left[Z\left((1 - \frac{b_m}{\upsilon}\right)\right] + \frac{a_m}{2.828 b_m RT}\left[\frac{b_i}{b_m} - \frac{2\sum_j x_j a_{ji}}{a_m}\right]\ln\left(\frac{1 + 2.414\frac{b_m}{\upsilon}}{1 - 0.414\frac{b_m}{\upsilon}}\right) \tag{18}$$

and when replacing υ in Eq.s (7a) and (7b) in term of ZRT/P, gives the cubic equation of SRK and PR-EOS in term of the compressibility factor (Z) as follow,

SRK-EOS:

$$Z^3 - Z^2 + \left(A + B - B^2\right)Z - AB = 0 \tag{19}'$$

PR-EOS:

$$Z^3 - (1 - B)Z^2 + \left(A - 2B - 3B^2\right)Z - \left(AB - B^2 - B^3\right) = 0 \tag{20}$$

A and B are defined as,

$$A = \frac{a_m P}{(RT)^2} \tag{21}$$

$$B = \frac{b_m P}{RT} \tag{22}$$

The design of separation processes strongly depend on accurate vapor–liquid equilibrium data. Extreme care must be exercised in choosing a model for phase equilibrium (some times called the fugacity coefficient, K-factor, or fluid model). Whenever possible, phase equilibrium data for the system should be used to regress the parameters in the model, and the deviation between the model predictions and the experimental data should be studied [10].

PHYSICAL PROPERTY CALCULATIONS

A. CHEMCAD

One of the major sections of any process simulation software is the physical properties and thermodynamic model selection. The physical property options are labeled as "thermo physical", "fluid package", or "databank" in common process simulators. CHEMCAD simulator data base included more than 1800 components, with more than 6000 binary data bank. Other sources for vapor-liquid equilibrium, in combination with mixing rules and more

than twenty thermodynamic models like PR , SRK, Henry, etc., provide the ideal means to easily model processes [11].

To use CHEMCAD Simulator as a physical property calculator, the following important steps can be used [11] :

1. Components specification, from ThermoPhysical Menu , Component List with their ID's are CO₂ (49), sulfolane (449), NMP (497), and PC (1799).User defined components were created by copying new components to make the editing of the binary interaction parameters (BIP) possible. Component List with their ID's became CO₂ (49), sulfolane (8001), NMP (8002), and PC (8003).

2. Selection of Thermodynamic Model, K-Values, PR or SRK, and editing the user defined BIP, From ThermoPhysical Menu, Databank , BIPS , enter constants A, B, and C. The BIP of the PR or SRK thermodynamic model may be correlated as a function of temperature with the following form:

$$k_{ij} = A_{ij} + B_{ij}T + C_{ij}T^2 \qquad \qquad \dots(23)$$

Where, k_{ij} is the binary interaction parameter between components i and j ,T :is the absolute temperature in K and A, B, and C are constants. All constants are not required, where if k_{ij} is constant (independent of temperature), then take k_{ij} equal to the constant A .

3.Plotting equilibrium data, from Menu Bar; Plot , TPxy options , select temperature and the two components required and range of plot.

B. HYSYS

The built-in property packages in HYSYS provide accurate thermodynamic, physical and transport property predictions for hydrocarbon, non-hydrocarbon, petrochemical and chemical fluids. The database consists of an excess of 1500 components and over 16000 fitted binary coefficients [12].

To use HYSYS Simulator as a physical property calculator, the following important steps can be used [12]:

1. Components selection, from the Simulation Basis Manager property view, the library component list and their ID's are CO₂ (14), sulfolane (978), NMP (446), and PC (606).

2. Selection of Thermodynamic Model, K-Values model, PR or SRK, and editing the user defined BIP directly from the Simulation Basis Manager property view, Fluid Packages. It does not need coped user defined components as in CHEMCAD.

3. Equilibrium Data, from Tools Bar; workbook-case, select temperature and the two components composition to get the equilibrium pressure. A table of equilibrium pressure vs. temperature can be constructed and plotted.

Process simulators provide an advice system for the selection of K-value and enthalpy methods, some time called wizard. It is no replacement for engineering judgment. The Wizard makes uses an algorithm based on general rules and may not always be correct. The suggested model may not be the 'best' model for the system [12].

RESULTS AND DISCUSSIONS

CHEMCAD and HYSYS simulators have been used to correlate the experimental solubility data of CO$_2$ in three physical solvents (sulfolane, PC, and NMP) at different temperatures (298.15 , 313.15, 323.15 , and 373.15 K) given by the literatures [1,2]. Two thermodynamic models PR and SRK were used.

A. CHEMCAD

Figure (1) illustrates the results of CO$_2$- Sulfolane system. SRK thermodynamic model, built in CHEMCAD simulator and used as such without modification (zero binary interaction parameters), gives results of small deviation (less than 5%) from the experimental data. Whereas PR thermodynamic model gave high deviation (higher than 20%).

Modifications of the thermodynamic models were performed on CHEMCAD simulator by editing user defined BIP of the systems used, especially which gives bad results and Table (2) shows the values of constants of the binary interaction parameter correlation in eq.(23) for the all binary systems studied and used in PR-model and SRK-model. Modified thermodynamic models for CO$_2$- sulfolane system of PR (k_{ij}= -0.001) give results of about 5% deviation. The values between brackets are the values of the BIP (k_{ij}). The very small value of the binary interaction parameter indicates some instability of PR thermodynamic model. Whereas modified thermodynamic models for CO$_2$- sulfolane system of SRK (k_{ij}=0.02) give results agree well to the experimental data, except for the temperature increases to 373.15 K, which correlated well at SRK (k_{ij}= 0).

Figure (2) shows the results of CO$_2$- PC system. The SRK thermodynamic model, used as such without modification (k_{ij}=0), gives results agree well to the experimental data for all temperature range used. Whereas PR (k_{ij}=0) thermodynamic model gave high deviation (

higher than 20%). Modified thermodynamic models for CO$_2$- PC system of PR (k_{ij}=-0.001) gives results of about 5% deviation. The very small value of the binary interaction parameter indicates some instability of PR thermodynamic model.

Figure (3) shows the results of CO$_2$-NMP system. Modified thermodynamic models of PR (k_{ij}= -0.001) gives results of about 5% deviation. The very small value of the binary interaction parameter indicates some instability of PR thermodynamic model. Whereas the thermodynamic model of SRK (k_{ij}=0) give results agree well to the experimental data, except for the temperature of 373 K, which correlated well at SRK (k_{ij}=0.02).

B. HYSYS

Modifications of the thermodynamic models were performed on HYSYS simulator by editing user defined BIP of the systems used, especially which gives bad results and Table (3) shows the values of constants of the binary interaction parameter correlation in eq.(23) for the all binary systems studied and used in PR-model and SRK-model.

Figure (4) shows the results of CO$_2$- sulfolane system. Modified thermodynamic models of PR (k_{ij}=-0.01), PR (k_{ij}= -0.02), and PR (k_{ij}=-0.03) at 298.15, 313.15, and 373.15K respectively, give results agree well to the experimental data, without noticing any instability as in the case of CHEMCAD. Whereas modified thermodynamic models of SRK (k_{ij}=-0.02), SRK (k_{ij}=-0.03), and SRK (k_{ij}=-0.04) at 298.15, 313.15 , and 373.15 K respectively, give results agree well to the experimental data.

Figure (5) shows the results of CO$_2$- PC system. Modified thermodynamic models of PR (k_{ij}=-0.02), PR (k_{ij}= -0.03), and PR (k_{ij}=-0.02) at 298.15 K, 313.15 K, and 373.15 K respectively, give results agree well to the experimental data, without noticing any instability as in the case of CHEMCAD. Whereas modified thermodynamic models of SRK (k_{ij}=-0.03), SRK (k_{ij}=-0.04), and SRK (k_{ij}=-0.04) at 298.15 K, 313.15 K, and 373.15 K respectively, give results agree well to the experimental data.

Figure (6) shows the results of CO$_2$-NMP system. Modified thermodynamic models of PR (k_{ij}=0.01), PR (k_{ij}=0), and PR (k_{ij}=0.03) at 298.15 K, 323.15 K, and 373.15 K respectively, give results agree well to the experimental data, without noticing any instability as in the case of CHEMCAD. Whereas modified thermodynamic models of SRK (k_{ij}=0.01), SRK (k_{ij}=0), and SRK (k_{ij}=0.02) at 298.15 K, 323.15 K, and 373.15 K respectively, give results agree well to the experimental data.

CONCLUSIONS

1. CHEMCAD simulator using the SRK model, used as such without modification (zero binary interaction parameters), gives a small deviation (less than 5%) . Higher deviation (about 10%) was noticed only for CO_2-NMP system at 373.15K.

2. CHEMCAD simulator using the PR model, used as such without modification, gives a high deviation (more than 20%) with all the three physical solvents systems. Modified thermodynamic models of PR (k_{ij} = -0.001) gives results of about 5% deviation. The very small value of the binary interaction parameter indicates some instability of PR thermodynamic model.

3. HYSYS simulator using the PR and SRK models, used as such without modification (k_{ij} = 0), gives deviations of about 10% ,without noticing any instability as in the case of CHEMCAD when modified.

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Table (1): Cubic equations of state used in present work [9].

SRK-EOS	PR-EOS
$P = \dfrac{RT}{\upsilon - b} - \dfrac{a}{\upsilon(\upsilon + b)}$ ...(7a) $a = a(T_c)\alpha(T_r, \omega)$ ...(8a) $\alpha(T_r, \omega) = \left[1 + \kappa\left(1 - T_r^{0.5}\right)\right]^2$ ...(9a) $\kappa = 0.48508 + 1.55171\omega - 0.15613\omega^2$ ...(10a) $a(T_c) = 0.42748\dfrac{(RT_c)^2}{P_c}$ ...(11a) $b = 0.08664\dfrac{RT_c}{P_c}$ ...(12a)	$P = \dfrac{RT}{(\upsilon - b)} - \dfrac{a}{\left[\upsilon(\upsilon + b) + b(\upsilon - b)\right]}$ ...(7b) $a = a(T_c)\alpha(T_r, \omega)$ ...(8a) $\alpha(T_r, \omega) = [1 + \kappa(1 - T_r^{0.5})]^2$ ...(9a) $\kappa = 0.37464 + 1.54226\omega - 0.26992\omega^2$ ...(10b) $a(T_c) = 0.45724\dfrac{R^2 T_c^2}{P_c}$ ...(11b) $b = 0.0778\dfrac{RT_c}{P_c}$ ...(12b)

Table (2): The values of constants of the binary interaction parameter correlation in eq.(23) when using CHEMCAD simulator.

System	PR-Model			SRK-Model		
	A	B	C	A	B	C
CO$_2$-Sulfolane	-0.001	0.000	0.000	-0.395	0.002	-0.000004
CO$_2$-PC	-0.001	0.000	0.000	0.000	0.000	0.000000
CO$_2$-NMP	-0.001	0.000	0.000	0.513	-0.003	0.000005

Table (3): The values of constants of the binary interaction parameter correlation in eq.(23) when using HYSYS simulator.

System	PR-Model			SRK-Model		
	A	B	C	A	B	C
CO$_2$-Sulfolane	0.811	-0.004	0.000007	0.801	-0.004	0.000007
CO$_2$-PC	1.216	-0.007	0.000010	0.998	-0.006	0.000009
CO$_2$-NMP	1.413	-0.008	0.000010	1.157	-0.007	0.000010
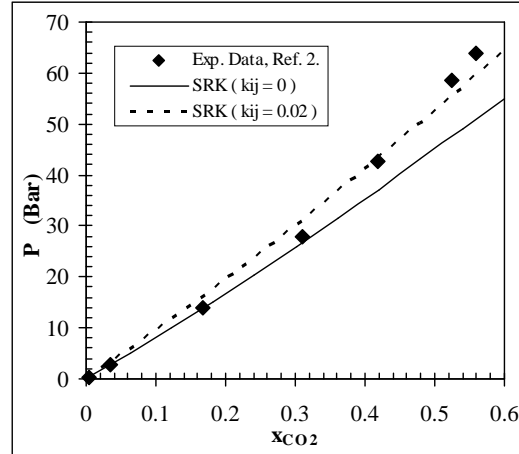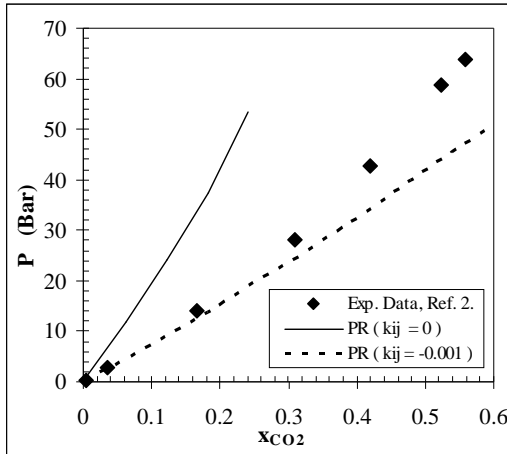
a. T=298.15K
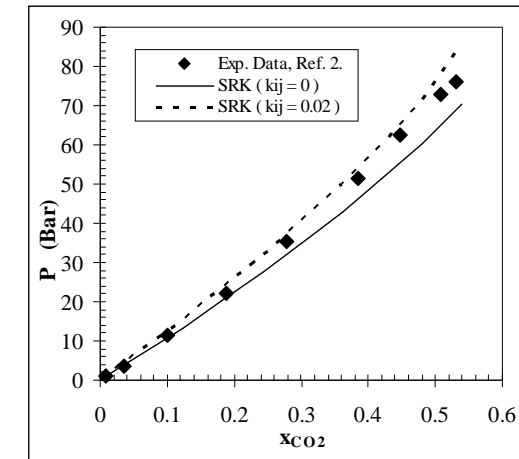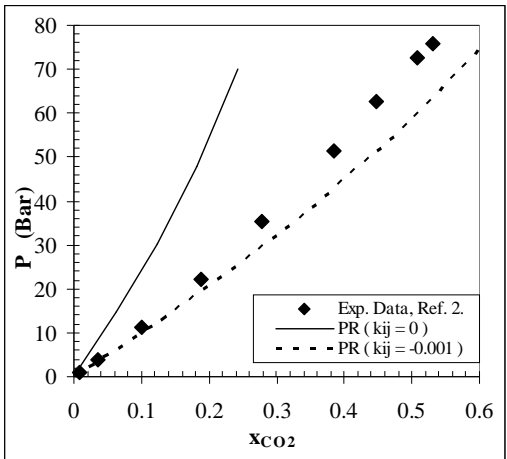
b. T=313.15K
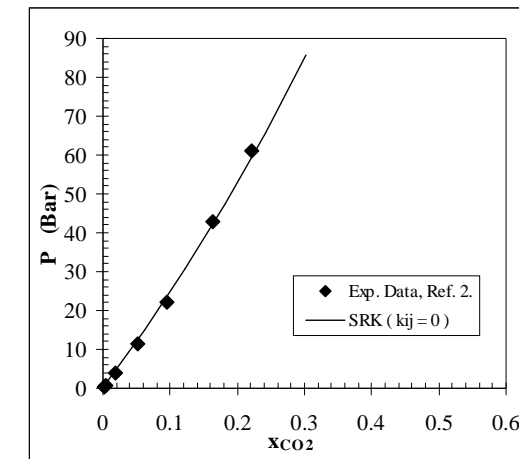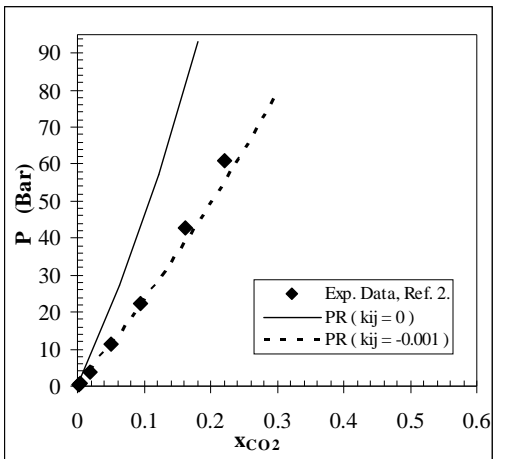
c. T=373.15K

Fig.(1): CHEMCAD mole fraction solubility of CO_2 in sulfolane at different temperatures by using PR- model and SRK-model.
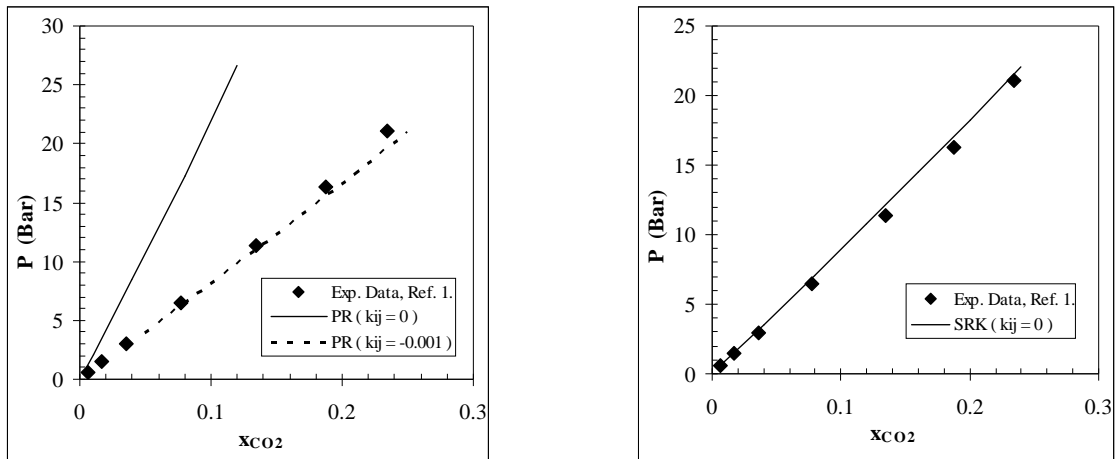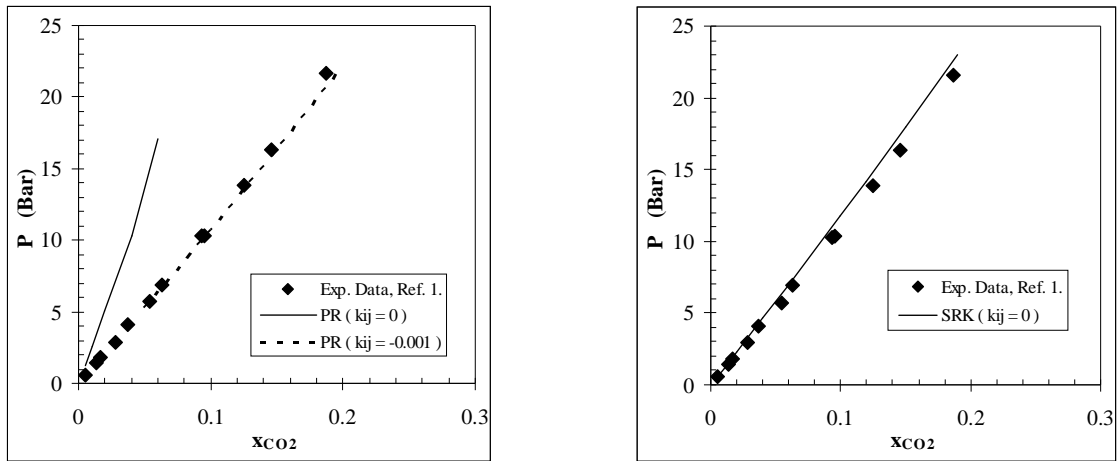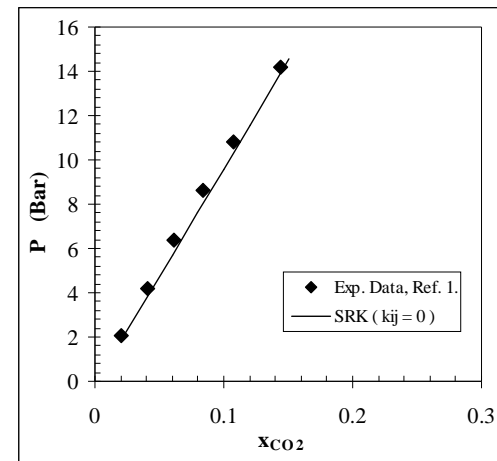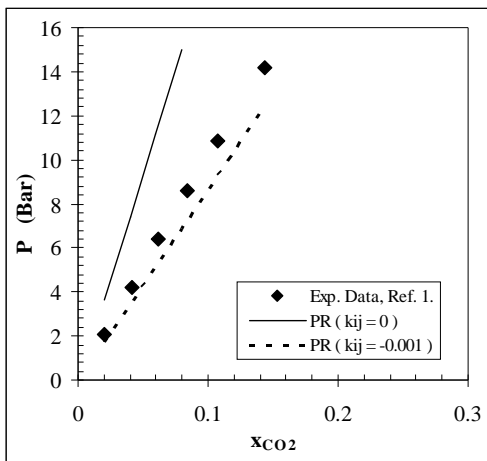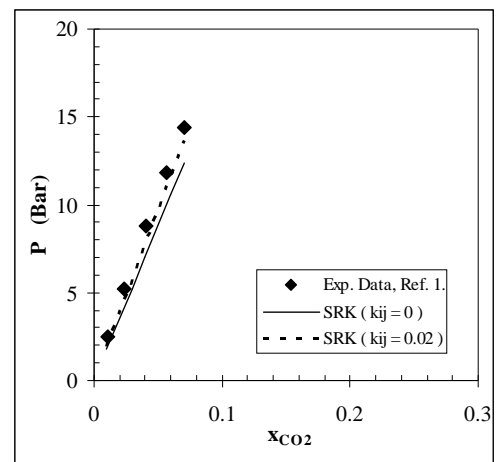
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b. T=313.15K
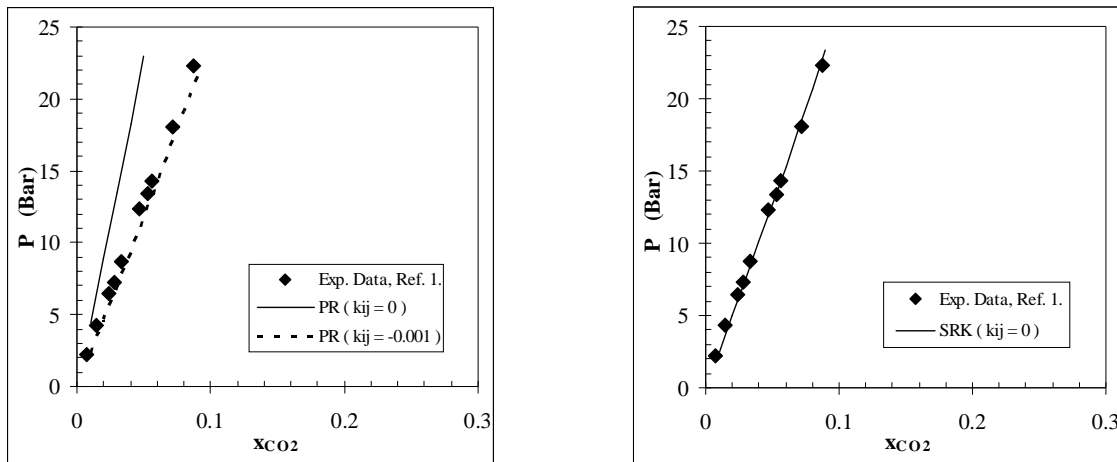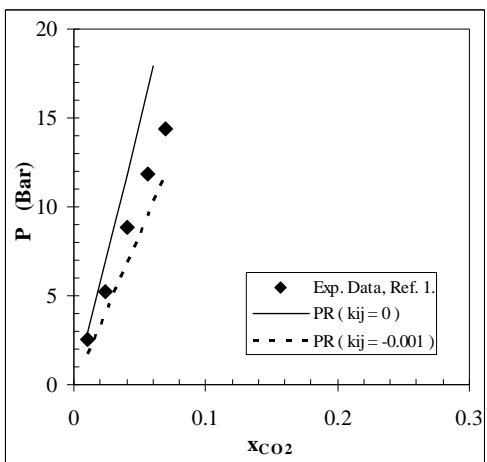

c. T=373.15K

Fig.(2): CHEMCAD mole fraction solubility of CO$_2$ in PC at different temperatures by using PR-model and SRK-model.
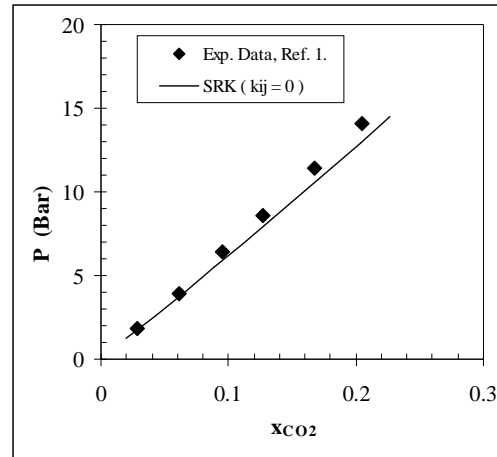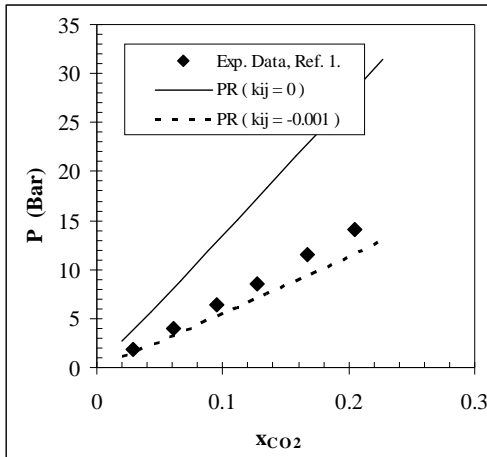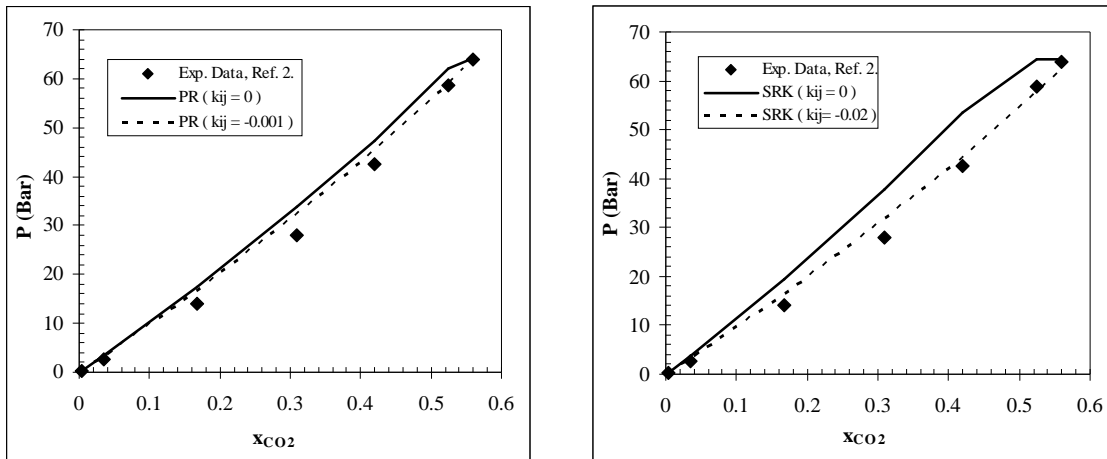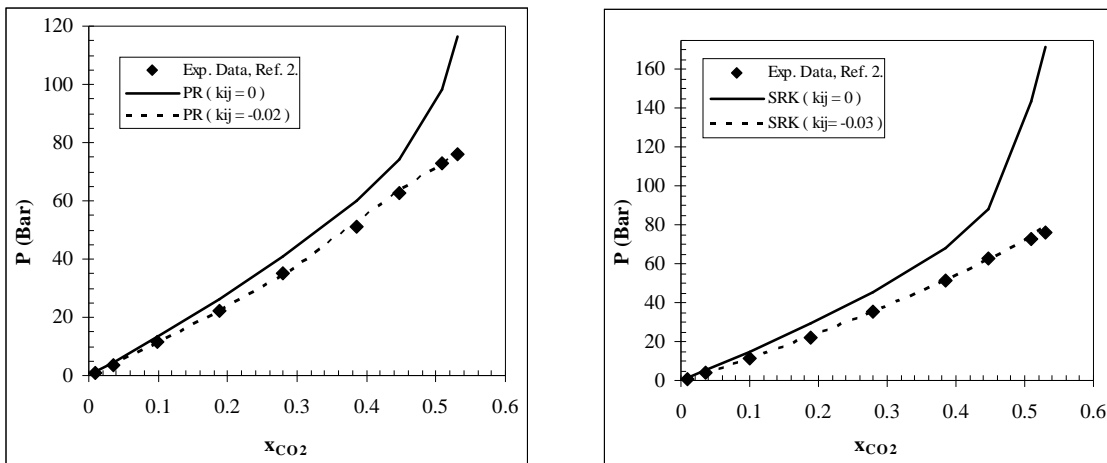
a.T=298.15K
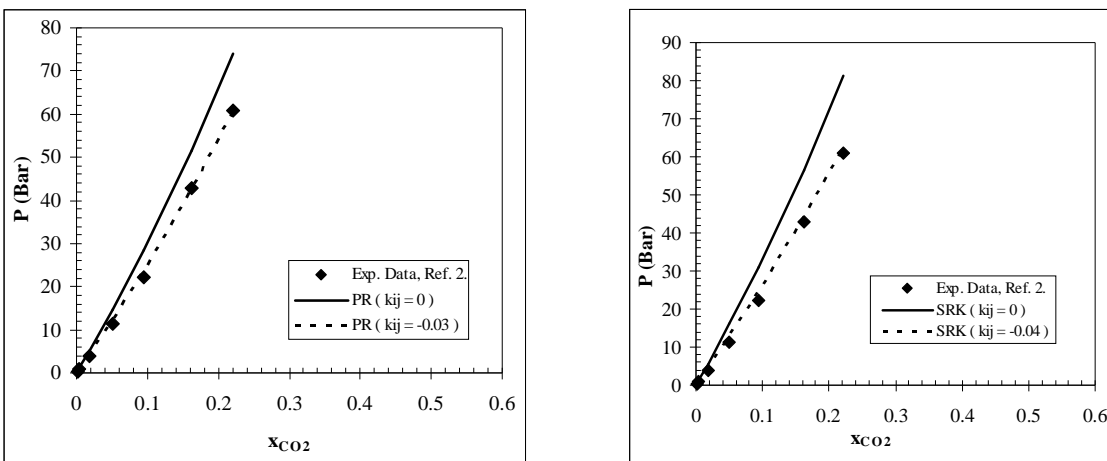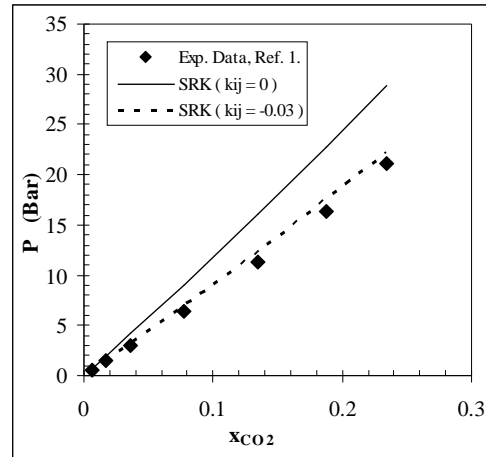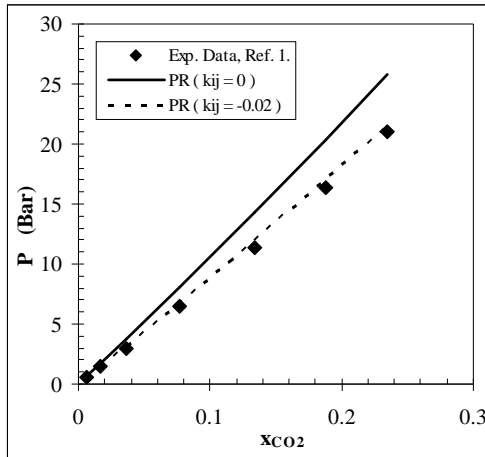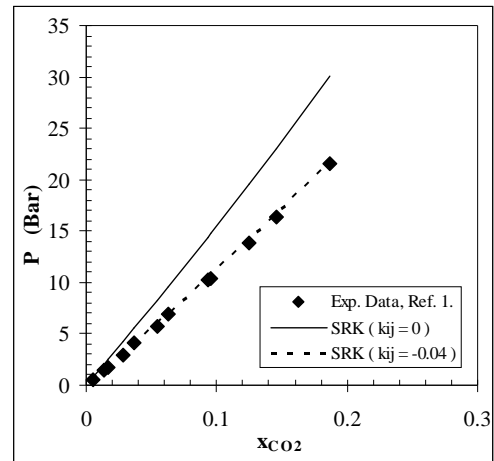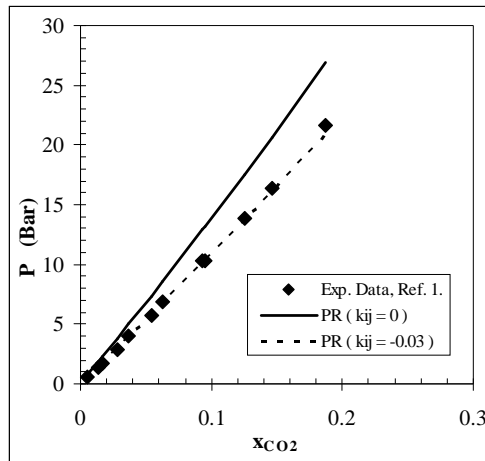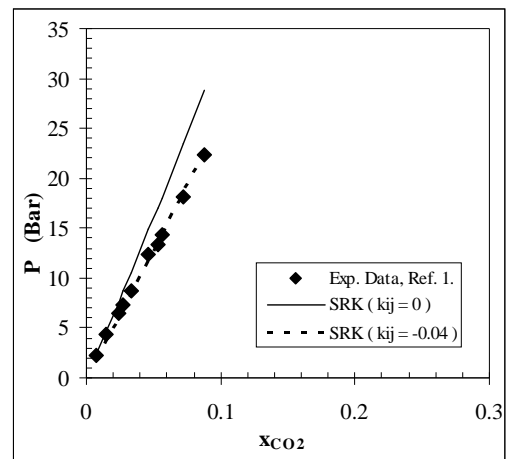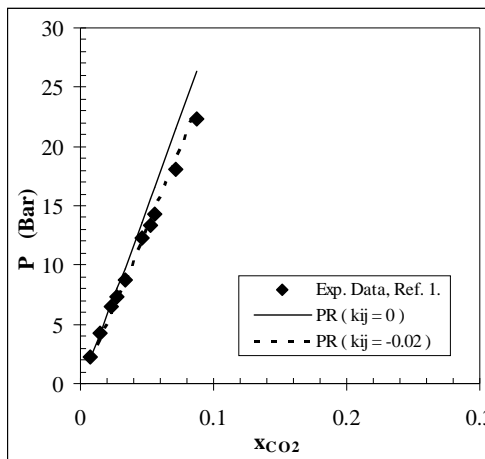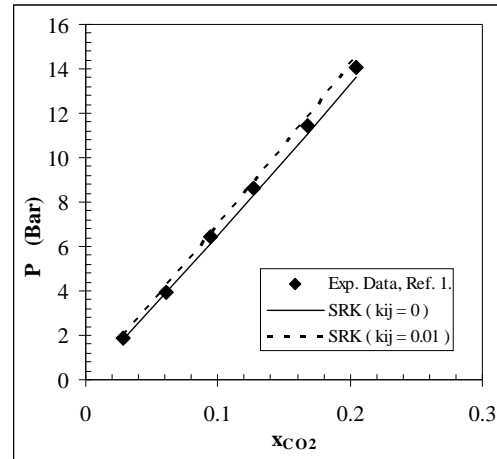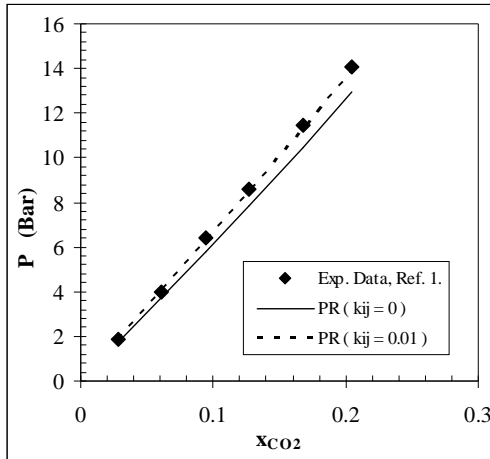

b. 323.15K

c. 373.15K

Fig.(3): CHEMCAD mole fraction solubility of CO$_2$ in NMP at different temperatures using PR – model and SRK-model.

a. T=298.15K

b. T=313.15K

c. T=373.15K

Fig.(4): HYSYS mole fraction solubility of CO$_2$ in sulfolane at different temperatures by using PR-model and SRK-model.
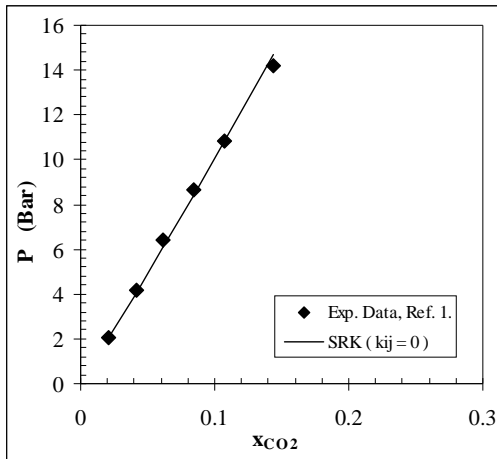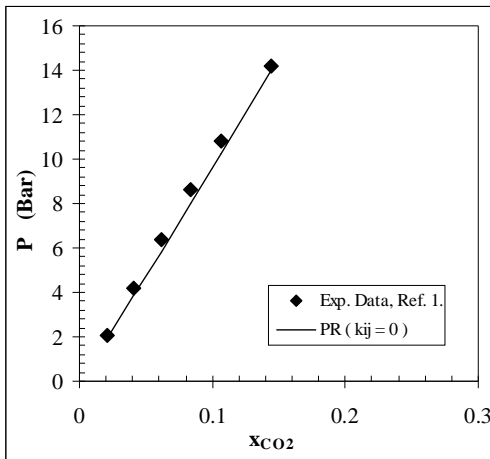
a. T=298.15K

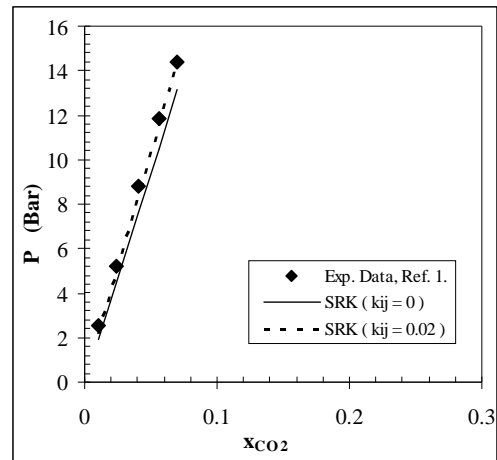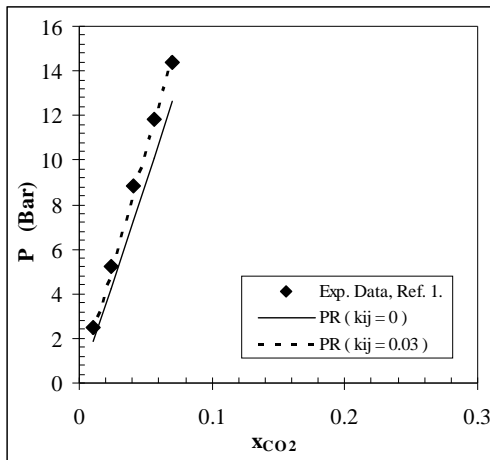b. T=313.15K

c. T=373.15K

Fig.(5): HYSYS mole fraction solubility of CO$_2$ in PC at different temperatures by using PR- model and SRK-model.

a. T=298.15K

b. T=323.15K

c. T=373.15K

Fig.(6): HYSYS mole fraction solubility of CO$_2$ in NMP at different temperatures by using PR-model and SRK-model.

تقدير ذوبانية غاز ثاني اوكسيد الكاربون في بعض المذيبات الفيزياوية السائلة باستعمال برنامجي المحاكاة CHEMCAD و HYSYS

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الخلاصة

استعمل برنامجي المحاكاة CHEMCAD و HYSYS لتحليل البيانات التجريبية المنشورة في الدوريات العلمية لذوبانية غاز ثاني اوكسيد الكاربون في عدد من المذيبات الفيزياوية السائلة وهي السلفولان (Sulfolane) والبروبلين كاربونيت (PC) والنورمل مثيل بايروليدون (NMP) في درجات حرارة مختلفة (298.15) و (313.15) و ( ) (323.15 و (373.15) كلفن . واستعمل موديلين لديناميك الحرارة وهما (PR) و (SRK).

إن نتائج برنامج CHEMCAD ولموديل (SRK) ، ولمعلومات اتزان الأطوار التجريبية للغاز مع جميع المذيبات الثلاثة ، وبدون أي تحسين للموديلين. أظهرت حيودا قليلا (بحدود 5%) . وأظهرت حيودا عاليا (10%) فقط مع الغاز و المذيب (NMP) عند ارتفاع درجة الحرارة إلى (373.15 K). أما نتائج الموديل (PR) ، ومن دون تحسين للموديل ، ولجميع المذيبات الفيزيائية الثلاثة، أظهرت حيودا عاليا (20%) . وعند تحسين موديلات ديناميك الحرارة بتصحيح قيمة معامل الترابط الثنائي للغاز مع المذيبات الثلاثة ، أعطت نتائج تطابق جيدة مع البيانات التجريبية ولكل من برنامجي المحاكاة CHEMCAD و HYSYS.

الكلمات الدالة: اتزان الأطوار غاز-سائل ، غاز ثاني اوكسيد الكاربون ، المذيبات الفيزيائية ، برامج المحاكاة ، CHEMCAD ، HYSYS ، موديلات ديناميك الحرارة ، معادلة الحالة.