THERMODYNAMIC MODEL FOR HIGH PRESSURE PHASE BEHAVIOR OF CARBON DIOXIDE IN SEVERAL PHYSICAL SOLVENTS AT DIFFERENT TEMPERATURES

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ABSTRACT

In the present study a thermodynamic model for prediction of gas-liquid equilibrium at high pressures and different temperatures prepared 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 Peng-Robenson equation of state (PR-EOS) with different mixing rules to show the effect of the type of mixing rule used.

Comparison of the experimental phase equilibrium data in the literature with the results of the model showed very good representation for some mixing rules and good for the others.

KEY WORDS: Gas-liquid equiliberium, carbon dioxide, liquid solvents,high pressure, Mixing rules,Peng-Robenson EOS.

NOTATIONS

a, b	parameters in the equation of state.
A, B	dimensionless parameters.
f	fugacity,bar.
k_{ij}, L_{ij}, H_{ij}	adjustable parameter.
n	number of components.
n_i	number of moles of component i, mole.
N	number of data points.
P	pressure, bar.
R	universal gas constant,lit. bar/ mole K.
T	temperature , K
x,y	liquid and gas mole fractions.
Z	compressibility factor.
$\underline{V}$	total system volume, lit.
v	total system molar volume , lit./mole.

Greek Symbols

$\hat{\phi}$	fugacity coefficient in mixture.

ω acentric factor.

Subscripts and Superscripts

c critical condition.

exp experimental value.

calc calculated value.

g gas phase.

ℓ liquid phase.

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. Because of their common structural feature, which is the puckered shape of the heterocyclic ring, intermolecular cavities are present in these structures that can accommodate the small cylindrical CO_2 molecules(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 ± 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 intraction 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 the 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.

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. Therefor the present work deals with the prediction of the gas-liquid equilibria of CO_2 with each of the liquid physical solvents sulfolane, NMP and PC at elevated pressures and different temperatures by a thermodynamic model used PR-EOS with different mixing rules to show the effect of the type mixing rule used on the results of model.

THERMODYNAMIC MODELING

The experiments that are done to obtain high-pressure phase-equilibrium data can be difficult and costly to perform. Hence, it is extremely useful to have a thermodynamic model or correlation scheme to extend and complement the experimentally obtained data for gas-liquid systems at high pressures.There is, however, one major problem associated with developing a reliable mathematical model of gas-liquid phase behaviour which is overcoming the difficality of description of interaction of molecules which differe in size, shape, or polarity. Although we have not completely overcome these difficulties in describing the phase behaviour, certain thermodynamic models will describe the high pressure phase behaviour in a qualitative(6) if not semiquantitative manner(7) .

Equation of State

Many models for supercritical-phase equilibria use an equation of state to calculate the fugacity of the component in the fluid phase. The results of these models are frequently very sensitive to the interaction energies and size factors, necessitating the need to develop improved mixing rules to estimate the mixture size and energy parameters needed in the equation of state. Cubic equations of state are exceedingly simple, have been remarkably successes in modeling phase behavior, and are probably the most widely used in analyzing experimental data(8). One of the cubic equation of state is the Peng and Robinson equation of state (PR-EOS) and the general form is (9):

$$P = \frac{RT}{(v-b)} - \frac{a}{v(v+b)+b(v-b)} \quad ..(1)$$

where,

$$a = 0.45724\frac{R^2T_c^2}{P_c}\alpha(T_r,\omega) \quad ....(2)$$

$(\alpha)^{0.5} = 1 + (1-T_r^{0.5})(0.37464 + 1.5422\omega - 0.2699\omega^2)$ … (3)

$$b = 0.0778\frac{RT_c}{P_c} \quad ....(4)$$

Replacing ν in Eq.(1) in term of ZRT/P, gives the cubic equation of compressibility factor as follow ,

$Z^3 - (1-B)Z^2 + (A-2B-3B^2)Z - (AB - B^2 - B^3) = 0$ ...(5)

A and B are defined as,

$$A = \frac{aP}{R^2T^2} = 0.45724\frac{P_r}{T_r^2} \quad ...(6)$$

$$B = \frac{bP}{RT} = 0.07780\frac{P_r}{T_r} \quad ...(7)$$

Table (1) shows the physical properties of components used in present work.

Mixing Rules for Equation of State

In order to obtain accurate properties of Gas-Liquid Equilibria (GLE), attention has been turned to calculate them from equations of state noting that those equations of state are strongly non-linear, needed effort and high computing time to be useful, as well as, these equations may deviate highly in case of non-ideal and polar systems. To overcome this problem efforts are directed to modify or improve mixing rules. In general an equation of state is develope first for pure component, then extended to mixtures through the use of mixing rules for combining the pure component parameters.

Most of simple equations of state are evolved from the van der Waal's mixing rules with or without modifications and the mixing rules for equation of state calculate the mixture parameters a_m and b_m for the equation of state according to the one-fluid mixing rules (Eqs. 8 and 9) and the only difference between them is the combining rule that determines how the cross coefficients a_{ij} and b_{ij} are calculated.

$$a_m = \sum_i^n \sum_j^n x_i x_j a_{ij} \qquad \text{….(8)}$$

and

$$b_m = \sum_i^n \sum_j^n x_i x_j b_{ij} \qquad \text{….(9)}$$

At this point, it should be made clear that all pure fluid parameters should have subscript (i) which was omitted for simplicity. Thus Eq.(4) may be written as follow,

$$b_i = 0.08664 \frac{RTc_i}{Pc_i} \qquad \text{…(10)}$$

The mixing rules used in present work are:

1.van der Waal's mixing rules (MR1):

$$a_m = \left[\sum_i^n \left(x_i a_i^{0.5} \right) \right]^2 \qquad \text{…(11)}$$

$$b_m = \sum_i^n x_i b_i \qquad \text{…(12)}$$

where a_i is given by

$$a_i = 0.45724 \frac{\alpha_i R^2 Tc_i^2}{Pc_i} \qquad \text{...(13)}$$

2.Modified van der Waal's mixing rules (MR2):

The value of $(a_i a_j)^{0.5}$ for many modifications is replaced by the cross parameter a_{ij}; and the binary interaction parameter k_{ij} may be introduced, as for the Peng-Robinson equation of state,

$$a_{ij} = (1 - k_{ij})\,(a_i\, a_j)^{0.5} \qquad \text{...(14)}$$

For an n-component mixture there are $\frac{n(n-1)}{2}$ possible binary interaction parameters.

All equations of state studied are extremely sensitive to the interaction energy and size factor of dissimilar components in the mixture. Therefore, the form of the mixing rules to obtain the mixture parameters becomes very important, and improving the mixing rules has been the object of extended research. In most cases, the improved mixing rules involve one or more additional adjustable parameters (such as k_{ij}).

3.Quadratic mixing rules (MR3) (10):

Quadratic mixing rule offers only two adjustable parameters per binary system. One binary interaction parameters is used to adjust the mixture parameter b_m, other parameters are used to adjust the mixture parameter a_m. Often, the quadratic mixing rule is sufficient for the correlation of equilibrium in systems that do not contain specific interactions. Mostly, the use of the second adjustable parameter L_{ij} is avoided, by setting all $L = 0$.

$$a_{ij} = \sqrt{a_i a_j}(1 - k_{ij}) \text{ with } k_{ji} = k_{ij} \quad ...(15)$$

and

$$b_{ij} = \frac{b_i + b_j}{2}(1 - L_{ij}) \text{ with } L_{ji} = L_{ij} \quad \mathbf{....(16)}$$

4.Panagiotopoulos-Reid Mixing Rule (MR4) (11):

The quadratic mixing rule (Eq.8) is often sufficient only for the correlation of equilibrium in systems where no specific interactions are involved. Panagiotopoulos and Reid (1985) have been the first to use two binary interaction parameters per binary system in order to fine-tune the parameter a. In most cases, the parameters L_{ij} are set to zero, because the use of k_{ij} and H_{ij} already allows excellent representations of much highly non-ideal binary phase equilibrium. The use of the two parameters k_{ij} and H_{ij} is much more powerful than the use of the two parameters k_{ij} and L_{ij} of the quadratic mixing rule. If all H are set to zero, the quadratic mixing rule is obtained again.

$$a_{ij} = \sqrt{a_i a_j}(1 - k_{ij}^{PR} + H_{ij}^{PR} x_i) \text{ with}$$

$$H_{ij}^{PR} = k_{ij}^{PR} - k_{ji}^{PR} = -H_{ji}^{PR} \quad ....(17)$$

and b_{ij} as in Eq.(16).

Binary Gas-Liquid Equilibrium

The most computationally straightforward and thermodynamically suitable method for calculating high-pressure phase behaviour is to choose an equation of state to model the equilibrium liquid phase and vapour phase. For the vapour-liquid equilibrium calculations, at equilibrium state the fugacities for all species i must be the same in all phases, namely,

$$\hat{f}_i^{g} = \hat{f}_i^{\ell} \text{ or } \hat{\phi}_i^{g} y_i = \hat{\phi}_i^{\ell} x_i \quad ...(18)$$

where $\hat{\phi}_i^{\ell}$ and $\hat{\phi}_i^{g}$ are the fugacity coefficients of component i in the liquid and vapour phases respectively. Since pressure-explicit equations of state are more common types and the useful relation for finding fugacity coefficients(12) is,

$$\ln \hat{\phi}_i = \frac{1}{RT}\int_{v}^{\infty}\left[\left(\frac{\partial P}{\partial n_i}\right)_{T,v,nj} - \frac{RT}{\underline{V}}\right]d\underline{V} - \ln Z \quad (19)$$

where $\underline{V}$ is the total system volume, n_i and n_j are the mole numbers of component i and j respectively.To calculate the fugacity coefficients, equations of state which are valid for both gas phase mixture and liquid phase mixture where used. Cubic equations of state such as the PR-EOS have become important tool in the area of phase equilibrium modeling, especially, for systems at pressures close to or above the critical pressure of one or more of these system components.

When the PR-EOS is introduced into the Eq. (19), the following closed-form expression for fugacity coefficient is obtained in the liquid phase,

$$\ln \hat{\phi} i = \frac{b_i}{b_m}(Z-1) - \ln\left[Z\left(1-\frac{b_m}{v}\right)\right] + \frac{a_m}{2.828RTb_m}\left(\frac{b_i}{b_m} - \frac{2}{a_m}\sum_j x_i a_{ij}\right)\ln\left(\frac{1+2.414\frac{b_m}{v}}{1-0.414\frac{b_m}{v}}\right) \tag{20}$$

where Z is the compressibility factor of the liquid mixture and may be calculated from the cubic equation (5) by an iteration method such as Newton-Raphson method.The fugacity coefficients of the components in the gas phase are also calculated with Eq.(20) with, y_i and all the (PR) a and b values for the gas replacing their corresponding terms.

RESULTS AND DISCUSSION

A major goal of the present study is the prediction of the gas-liquid equiliberium of binary system by a thermodynamic model using PR-EOS which needs only the physical critical properties of the pure components and using different mixing rules without and with one or more adjustable parameters.Therefor the adjustable parameters can be determined by fitting an experimental data of mole fraction solubilities of CO_2 in liquid solvent which are obtained from the available literture with the equation of state used by a series of values of adjustable parameters assumed and the mole fraction solubilities of CO_2 are calculated for each isotherm pressure.The accepted values of adjustable parameters are that which gives the minimum percentage of mean absolute deviation (%MAD) defined as follow,

$$\%MAD = \frac{100}{N}\sum\left|x_{\exp.} - x_{calc.}\right| \qquad ...(21)$$

where N is the number of data points.The steps of the calculations and the computer program in basic language are described in details by Hadi $^{(13)}$.

The mole fraction solubilities of CO_2 in sulfolane, NMP , and PC solvents are measured experimentally by Murrieta et al., Jou et al. and Robert and Mather,(1,2,4).The data of these literture are fitted with the PR-EOS using different mixing rules to get values of adjustable parameters for each mixing rule at each temperature.The results are listed in Table (3) for the all binary systems studied. For all mixing rules at each temperature the %MAD's between the predicted and the experimental data for all systems are shown in Table (4).

The values of adjustable parameter k_{12} in MR2 decreased as the temperature is increased , but it's values are osillated in MR3 and MR4 for all systems studied. The values of L_{12} in MR3 decreased with the temperature increased for the CO_2-NMP system and it's values are osillated with the temperature increased for other systems.The values of H_{12} in MR4 are osillated with the temperature increase for all systems as shown in Table (3) and this due to the calculations dependence on the data in liquid phase only. Therefor, the relation form between the temperature and the values of adjustable parameters in all the mixing rules taken can not be determined correctely and it requires additional experimental data for the gas –liquid equilibrium.

The mixing rules MR3 and MR4 gave %MAD smaller than the mixing rules MR1 and MR2 and the MR3 gave %MAD less than the MR4 for all systems studied as shown in Table (4). Thus, the MR3 with two adjustable parameter k_{12} and L_{12} can be used to calculate the gas-liquid equilibrium of CO_2 (1)-liquid solvent (2) at high pressures and different temperatures adequately.

The determined values of adjustable parameters are used to predict the gas-liquid equiliberium of CO_2 (1)-liquid solvent (2) and are shown graphically in Figs (1-11). The systems form "open loop" pressure composition diagram and the gap of loops increased with temperature increased because of the system pressure close to and above the critical pressure of one of these system components. Any detailes of gas-liquid equiliberium calculations and other graphs for the other temperatures are described in ref (13).

Comparison of the results of the model with the experimental phase equilibrium showed very good representation for the mixing rules MR3 and good for the other mixing rules.

CONCLUSIONS

1. It is possible to collate gas-liquid equiliberium of CO_2 – liquid solvent system adequately by using PR-EOS with the mixing rules of two adjustable parameters.

2. The MR3 with two adjustable parameter k_{12} and L_{12} can be used to calculate the gas -liquid equilibrium of CO_2 (1)-liquid solvent (2) at high pressures and different temperatures because it gave high accuracy compared with the other mixing rules.

3. The relation form between the temperature and the values of adjustable parameters in all mixing rules can not be determined correctely due to the osillation of adjustable parameters values with changing temperature except the CO_2-sulfolane system can be said the relation is linear.

4. Comparison of the results of the model with the experimental phase equilibrium showed very good representation for the mixing rules MR3 and good for the other mixing rules.

5. The systems form "open loop" pressure composition diagram and the gap of loops increased with temperature increased because of the system pressure close to and above the critical pressure of one of these system components.

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Table (1): Physical properties of components studied. [(12)]

Component	Chemical form	Tc (K)	Pc (bar)	ω
Carbon dioxide	CO_2	304.7	73.8	0.225
Sulfolane	$C_4H_8SO_2$	849.6	50.3	0.378
NMP	C_5H_9NO	724.1	47.8	0.356
PC	$C_4H_6O_3$	775.4	54.1	0.434

Table(2): The mixing rules equations used in present work .

No	Mixing rules	Adjustable parameters
1	$a_m = \left[\sum_i^n (x_i a_i^{0.5})\right]^2$ and $b_m = \sum_i^n x_i b_i$ $a_{ij} = \sqrt{a_i a_j}$	k_{12}=0
2	$a_m = \sum_i^n \sum_j^n x_i x_j a_{ij}$ and $b_m = \sum_i^n x_i b_i$ $a_{ij} = (1-k_{ij})(a_i a_j)^{0.5}$	k_{12}=value.
3	$a_m = \sum_i^n \sum_j^n x_i x_j a_{ij}$ and $b_m = \sum_i^n \sum_j^n x_i x_j b_{ij}$ with $a_{ij} = (1-k_{ij})(a_i a_j)^{0.5}$ and $b_{ij} = \frac{b_i + b_j}{2}(1 - L_{ij})$	k_{12} =value , L_{12} = value.
4	$a_m = \sum_i^n \sum_j^n x_i x_j a_{ij}$ and $b_m = \sum_i^n \sum_j^n x_i x_j b_{ij}$ with $a_{ij} = \sqrt{a_i a_j}(1 - k_{ij}^{PR} + H_{ij}^{PR} x_i)$ and $b_{ij} = \frac{b_i + b_j}{2}(1 - L_{ij})$	k_{12}=value, L_{12} = value, H_{12}=value.

Table(3):Adjustable parameters values obtained by fitting with PR-EOS.

T (K)	MR1	MR2	MR3		MR4			Ref.
	k_{12}	k_{12}	k_{12}	L_{12}	k_{12}	L_{12}	H_{12}	
CO_2(1) – Sulfolane(2)								
298.15	0	0.0287	0.0101	0.0851	0.0173	0.0851	0.0163	2
313.15	0	0.0237	0.0240	-.0031	0.0237	-0.0031	-0.0008	2,5
343.15	0	0.02475	0.0134	0.0686	0.0010	0.0686	-0.0516	2
373.15	0	0.0187	0.0072	0.0666	0.0023	0.0666	-0.0313	2,5
403.15	0	0.0139	0.0022	0.1532	-0.00075	0.1532	-0.0231	2
CO_2(1) – NMP(2)								
298.15	0	0.0128	0.0085	0.0755	0.0092	0.0755	0.0054	1
323.15	0	0.0101	0.0111	-.0215	0.0166	-0.0215	0.0568	1
373.15	0	0.0037	0.0666	-0.911	0.0465	-0.9110	-0.3915	1
CO_2(1) – PC(2)								
298.15	0	0.0068	0.0059	0.0158	0.0095	0.0158	0.0217	1
313.15	0	0.0047	0.0027	0.0312	0.0065	0.0321	0.0336	1
373.15	0	0.0163	0.0325	-.3506	0.0247	-0.3506	-0.1435	1

Table(4):%MAD between the experimental and predicted mole fraction solubilities of CO_2 in solvents using PR-EOS with different mixing rules.

%MAD					
T (K)	MR1	MR2	MR3	MR4	Ref.
CO_2(1) – Sulfolane(2)					
298.15	7.226	0.461	$1.19*10^{-3}$	$2.29*10^{-3}$	2
313.15	4.51	$7.27*10^{-2}$	$6.76*10^{-5}$	$5.22*10^{-4}$	2,5
343.15	2.32	0.121	$1.4*10^{-5}$	$8.38*10^{-4}$	2
373.15	0.606	0.186	$1.01*10^{-4}$	$5.72*10^{-4}$	2,5
403.15	0.541	$7.78*10^{-2}$	$1.18*10^{-4}$	$3.72*10^{-5}$	2

Table(4): continued

$CO_2(1)$ – NMP(2)					
298.15	1.03	$1.424*10^{-2}$	$6.021*10^{-5}$	$1.36*10^{-5}$	1
323.15	0.492	$4.04*10^{-3}$	$5.7*10^{-5}$	$9.32*10^{-5}$	1
373.15	0.863	$3.68*10^{-2}$	$2.63*10^{-4}$	$1.18*10^{-5}$	1
$CO_2(1)$ – PC(2)					
298.15	0.566	$2.94*10^{-2}$	$1.688*10^{-5}$	$5.78*10^{-7}$	1
313.15	0.247	$3.33*10^{-3}$	$1.17*10^{-6}$	$1.93*10^{-5}$	1
373.15	0.475	$7.107*10^{-3}$	$1.302*10^{-5}$	$2.66*10^{-5}$	1

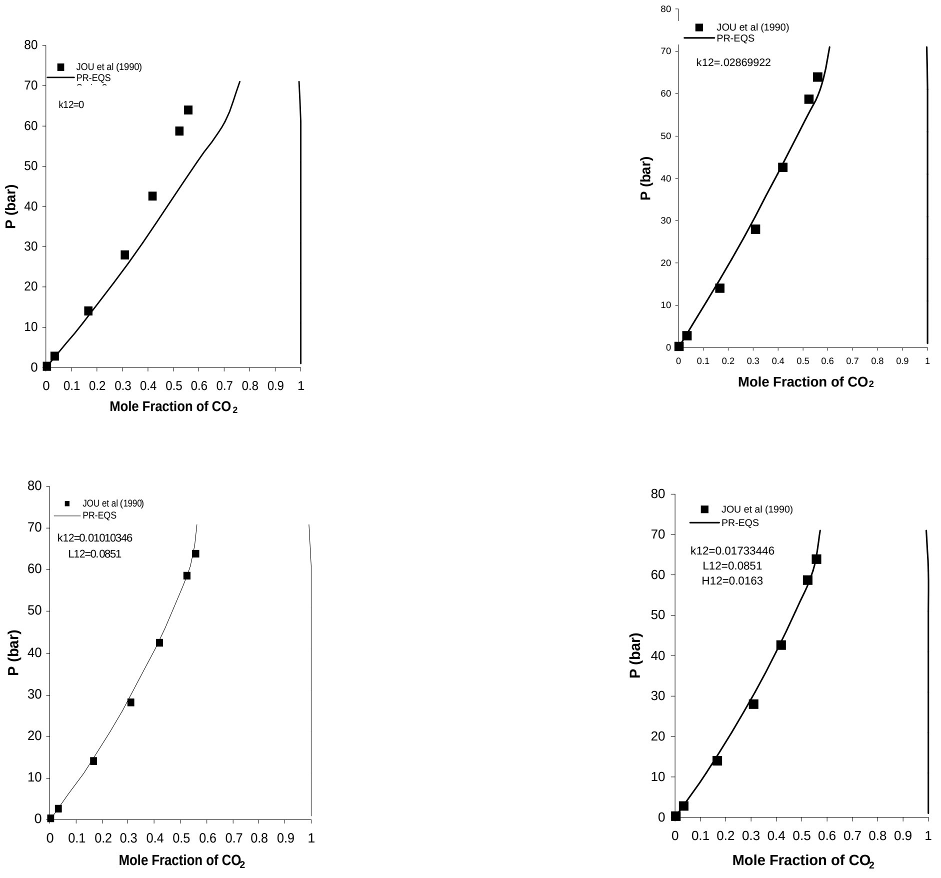

Fig.(1).Pressure-equilibrium phase composition diagram of CO_2-sulfolane system at 298.15 K.

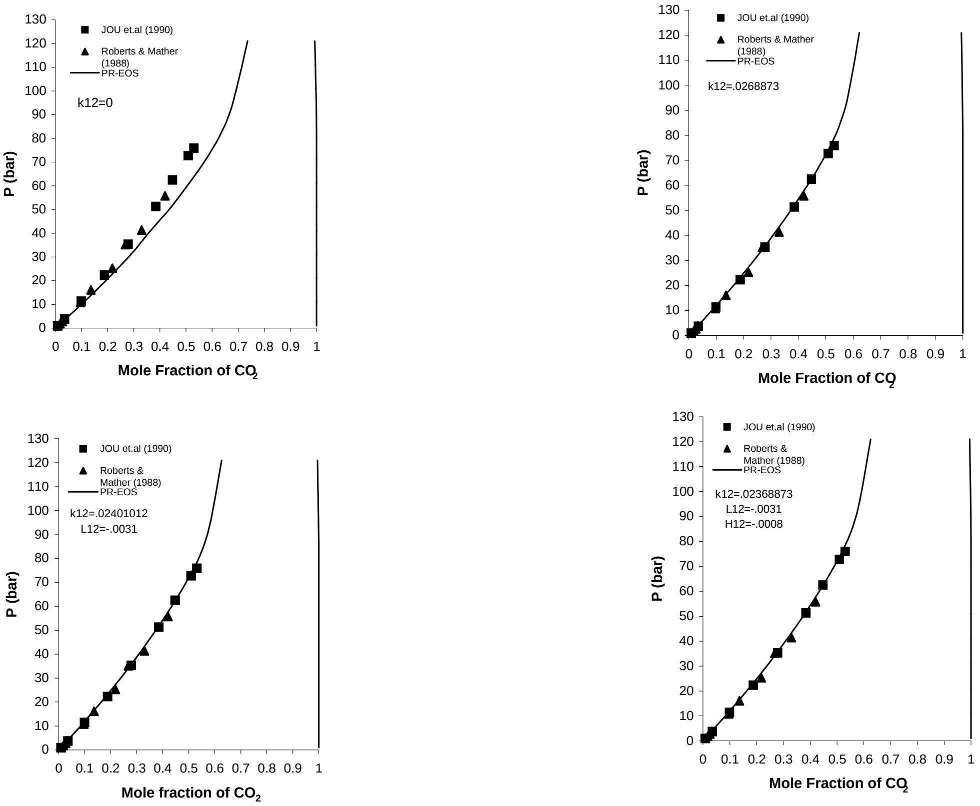

Fig.(2).Pressure-equilibrium phase composition diagram of CO_2-sulfolane system at 313.15 K.

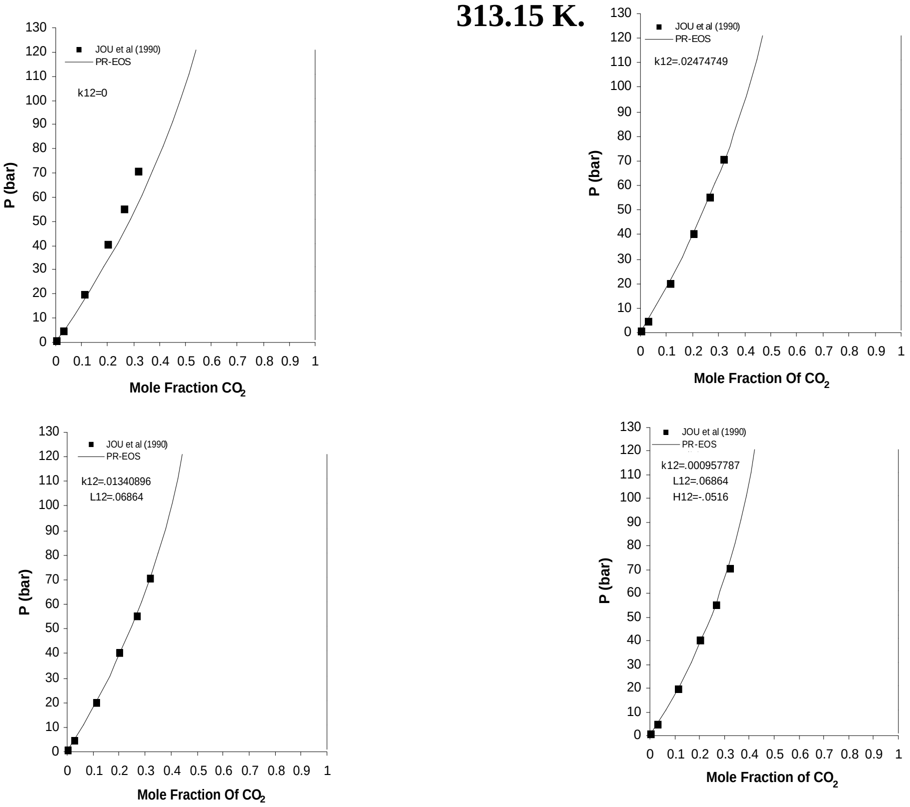

Fig.(3).Pressure-equilibrium phase composition diagram of CO_2-sulfolane system at 343.15 K.

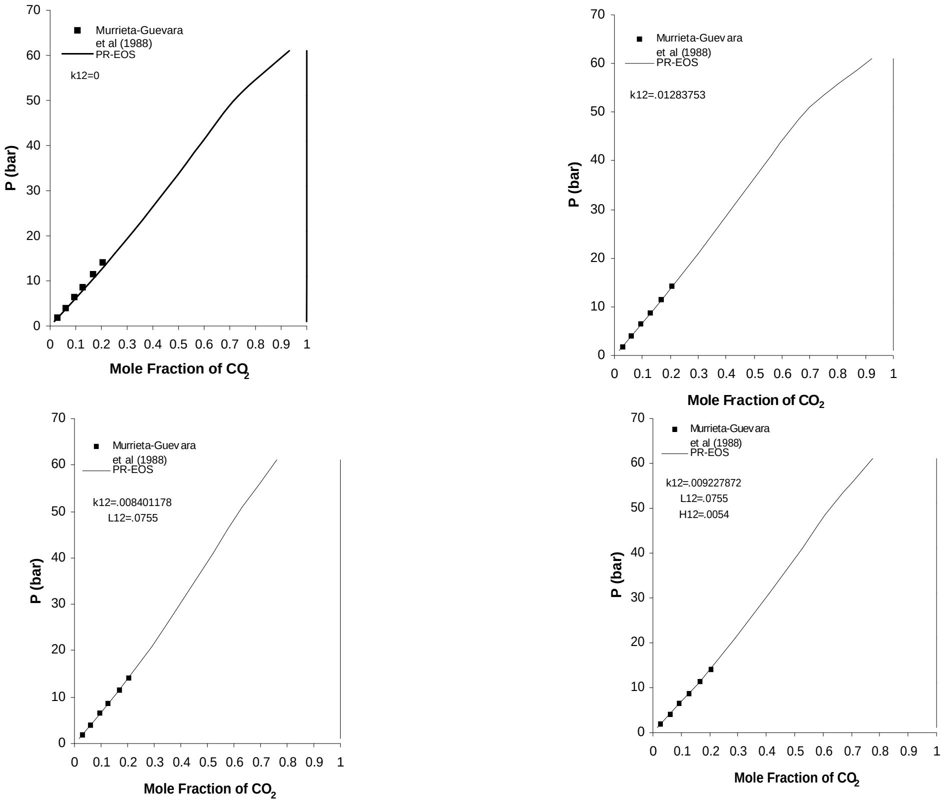

Fig.(6).Pressure-equilibrium phase composition diagram of CO_2-NMP system at 298.15K.

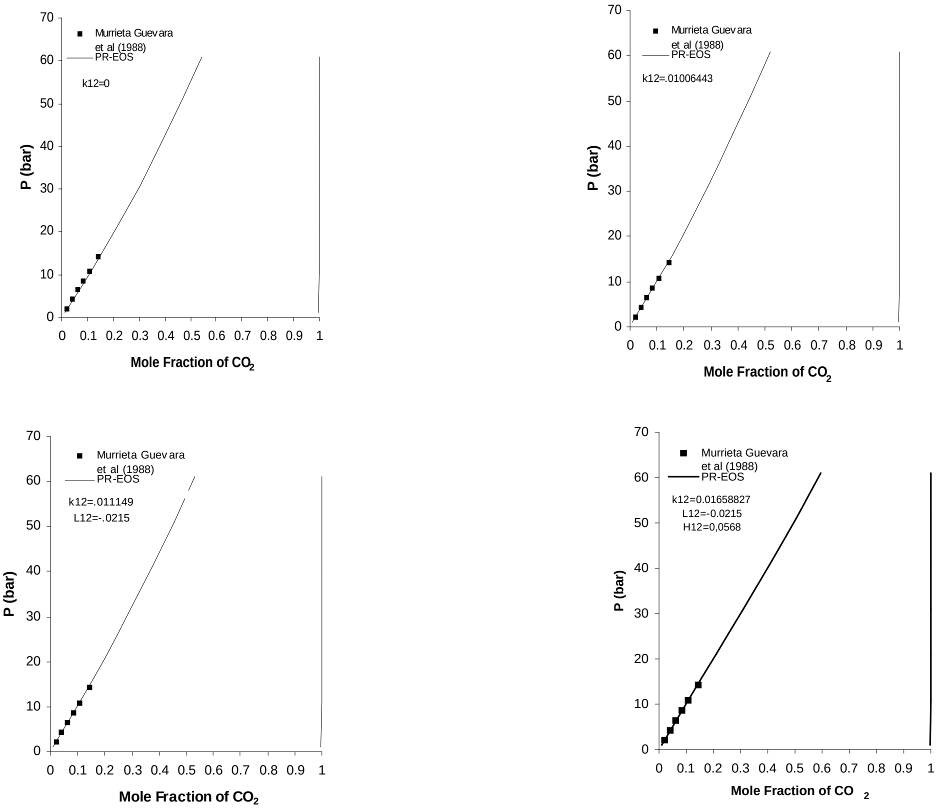

Fig.(7).Pressure-equilibrium phase composition diagram of CO_2-NMP system at 323.15 K.

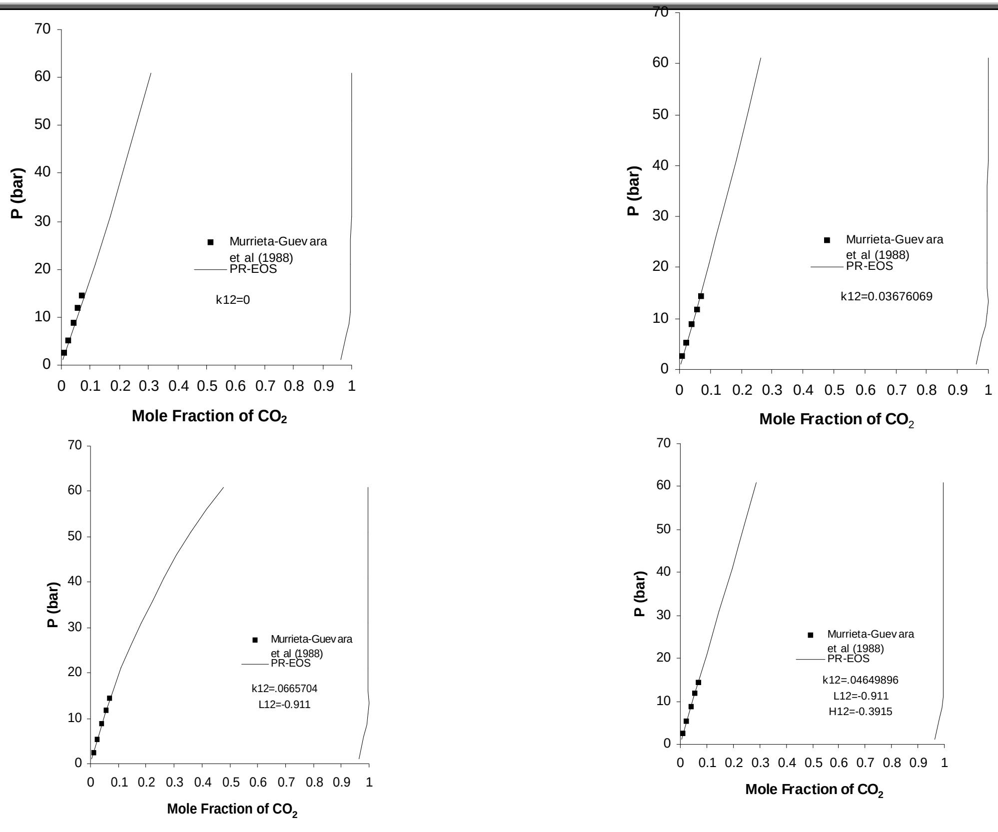

Fig.(8).Pressure-equilibrium phase composition diagram of CO_2-NMP system at 373.15 K.

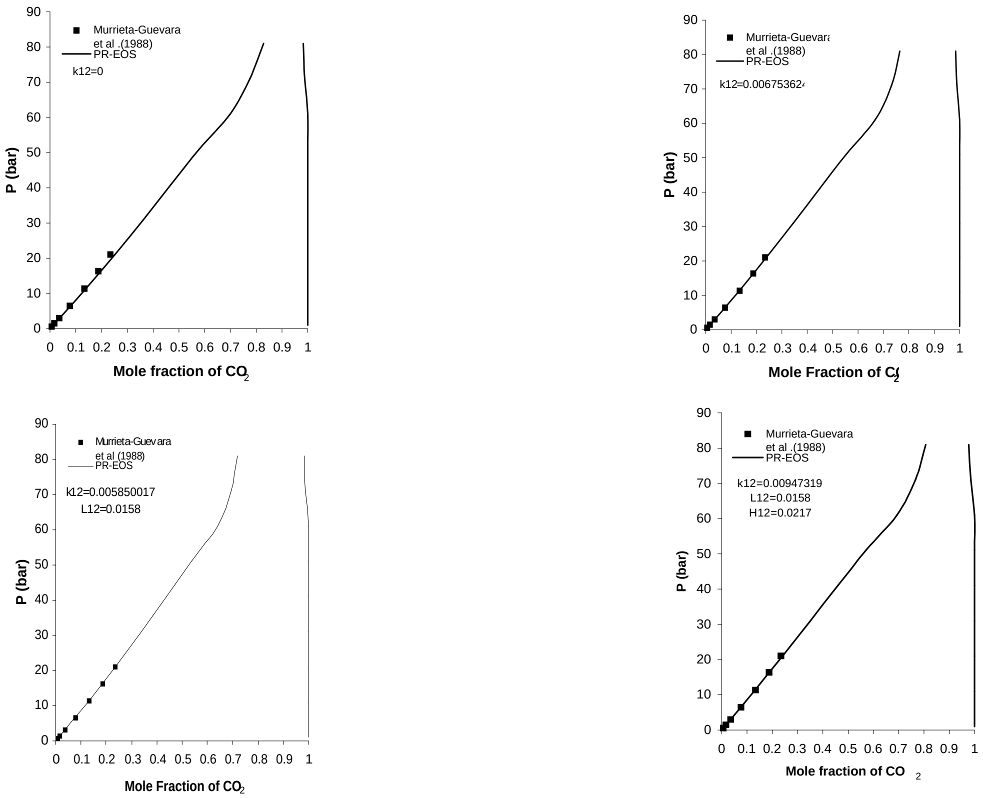

Fig.(9).Pressure-equilibrium phase composition diagram of CO_2-PC system at 298.15K

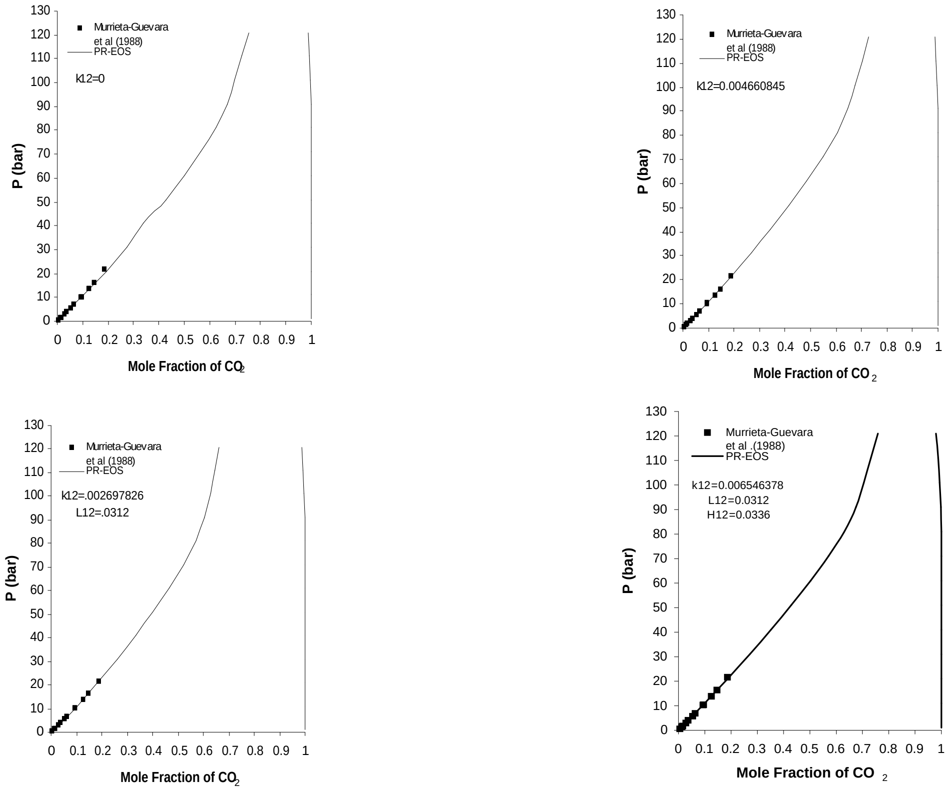

Fig.(10). Pressure-equilibrium phase composition diagram of CO_2-PC system at 313.15 K.

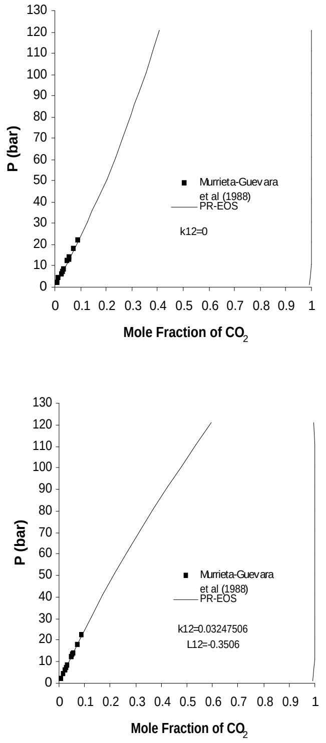

Fig.(11).Pressure-equilibrium phase composition diagram of CO_2-PC system at 373.15 K.

نمذجة في ديناميك الحرارة للسلوك الطوري لثاني أوكسيد الكاربون مع بعض المذيبات الفيزيائية السائلة لدرجات حرارة مختلفة (عند الضغوط العالي)

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الخلاصة

تم إعداد نموذج لاتزان غاز-سائل للأنظمة الثنائية في الضغوط العالية وعند درجات حرارة مختلفة لثاني أوكسيد الكاربون بثلاث مذيبات سائلة (سولفولان ونورمل مثيل بايروليدون وبروبيلين كاربونيت) بإستعمال معادلةَ بنك-روبنسون للحالة وقوانين خلط (mixing rules) مختلفة .

قورنت نتائج النموذج مع نتائج تجريبية تم الحصول عليها من المصادر والبحوث وقد تبين بان النموذج يعطي توافقا جيد جدا لبعض قوانين الخلط وجيد نوعا ما للبعض الآخر.

الكلمات الدالة: توازن غاز-سائل قوانين خلط ثاني اوكسيد الكاربون مذيبات سائلة ضغوط عالية معادلة بنك-روبنسون للحالة.