

A PHASE BEHAVIOR COMPOSITIONAL MODEL FOR JAMBOUR CRETACEOUS OIL RESERVOIR

Me'ad I. Al-Howaidi, Ghazwan N. Saad*, and Muhanad Abdul Rasak**

Petroleum Engineering Department – College of Engineering – University of Baghdad – Iraq

* Civil Engineering Department – College of Engineering – University of Kofa - Iraq

** Chemical Engineering Department – College of Engineering – University of Tikrit - Iraq

ABSTRACT

A computer phase behavior compositional model is developed "MIS-MODEL", that incorporate Modified Soave Redlich Kwong (M.S.R.K) & Pengrobinson (P.R.) equations of state. Tuning of the equations of state with the available experimental data is carried out. New interaction coefficients for Jambour oil reservoir are obtained for P. R.-E. O. S.

INTRODUCTION

The term phase is defined as: "any homogeneous and physically distinct part of a system with definite boundary surface ⁽¹⁾" definition of phase can be carried further depending on the degree of freedom.

The manner in which hydrocarbons behave when pressure and temperature are changed is explained best by consideration of the behavior of individual molecules which dependent on the three factors (pressure, temperature, molecule attraction and repulsion).

Phase can exist together in equilibrium. In this case all factors or variables that control the system are balanced or neutralized. The common forces or variables that control equilibrium or bring about phase change are temperature, pressure and composition.

Phase rule that was showed by the American Chemist J. Willard Gibbs a century ago, was that at equilibrium the equation $F = C - P + 2$ is obeyed*. This rule is useful as a quantitative check on whether a system is at equilibrium and allows elucidation and manipulation of complex phase relation.

There are three kinds of hydrocarbon system (single, binary and multi components) each one of these has special features and behavior under various condition of pressure and temperature. In order to describe the phase behavior of hydrocarbon system, some tools are used to

explain the behavior of phases under certain condition which include:

- P-V diagrams.
- P-T diagrams.
- P-Z diagrams.
- Z-Z diagrams (Pseudo-ternary diagrams).

Each of the above tools can display a side of interest explanation. For example, if the interest is with phase behavior during miscible displacement, the best tools is "Pseudo-ternary diagram" that use the compositions to indicate points which represent mixtures of components and their state under certain pressure and temperature.

McCain, W. D. ⁽¹⁾ (1990) divided hydrocarbon fluids into five types according to (P-T) diagram of each type. These are: black oils, volatile oils, retrograde gases, wet gases and dry gases.

Methods for Calculating Vapor/Liquid Equilibrium

Vapor/liquid equilibrium which is pressure, temperature composition dependent, i.e. $k = f(P, T, Z)$ has many methods of calculation. McGlashan, R. S. (1980) ⁽²⁾ displayed some of the criteria that were used to select a suitable method for calculating k values for petroleum engineering application.

Methods of calculating equilibrium ratio for use in petroleum engineering application have been reviewed by Peden, J. (1976) ⁽³⁾. The

*Where F = number of degree of freedom, C = number of component in each phase & P = number of phases.

following classification of methods were proposed:

1. Methods which involve empirical curve fitting of K-values such as NGPA* K-values charts that required a convergence pressure which accounts for the composition effect on phase equilibrium.
2. Methods derived from thermodynamic principles. Peden J. ⁽³⁾ (1976) and McGlashane R. ⁽²⁾ (1980) classify these methods into:
 - a. Methods based on the principle of corresponding state (P. C. S.).
 - b. Methods based on molecular thermodynamics.
 - c. Methods based on semi-empirical equations of state.

Vapor/Liquid Equilibrium Theory

The thermodynamic fundamentals of phase behavior were first developed by Gibbs (1877), he established that (a vapor and liquid are in equilibrium if and only if their pressure and temperature are identical and Gibbs free energy of the system is a minimum). The Gibbs free energy is defined by:

$$G = H - TS \quad (1)$$

Where (H = enthalpy, S = entropy) of system. By considering a multi-component fluid where the number of moles of the component (i) is given by N_i^L and N_i^V , the criteria that the Gibbs free energy is a minimum is satisfied when:

$$\partial G / \partial N_i^L - \partial G / \partial N_i^V = 0 \quad (2)$$

The partial derivatives $\partial G / \partial N_i^L$ and $\partial G / \partial N_i^V$ are by definition the chemical potentials of components i in the liquid and the vapor phases respectively, denoted by U_i^L and U_i^V . Thus the condition for thermodynamic equilibrium can also be expressed as an equality of chemical potentials.

$$U_i^L = U_i^V \quad (3)$$

It can be shown from basic thermodynamic principles that at constant temperature, the change in G with pressure is given by:

$$dG = V dp \quad (4)$$

and applying this to the definition of chemical potential gives:

$$dU_i = V_i dp \quad (5)$$

where V_i = the partial molar volume of component i defined by:

$$V_i = \partial V / \partial N_i \quad (6)$$

Equations (5) and (6) are valid for either liquid or vapor phases. For an ideal gas Equation (5) and (6) can be combined with the general gas law to give:

$$dU_i = R T d(\ln P_i) \quad (7)$$

Where P_i is the partial pressure of component i when a system is not ideal, a new quantity called fugacity (f_i), is introduced in order to preserve the simple form of Equation (7) as:

$$dU_i = R T d(\ln f_i) \quad (8)$$

For a two phase system to be in equilibrium, the chemical potentials in the two phase must be equal and it follows that the fugacities must also be equal.

$$f_i^L = f_i^V \text{ for all } i \quad (9)$$

The fugacity has units of pressure and may be thought of as a partial pressure corrected for non-ideal behavior. In an ideal gas the fugacity is equal to the partial pressure. As will be shown later, fugacity of component or fugacity coefficient is an important parameter that is calculated from the equation of state in predicting k-value for each component. To simplify the equation that is useful to define fugacity coefficient ϕ_i , is given by:

$$f_i^L = \phi_i^L X_i P \quad (10)$$

$$f_i^V = \phi_i^V Y_i P \quad (11)$$

Where X_i , Y_i are the mole fraction of component i in liquid and vapor phases respectively. Then using Equations (4) and (5) in combination with the general gas law gives:

*Natural Gas Process Association.

$$\ln(\phi_i/\phi_i^0) = \int_{P_0}^0 (1/RT)(\partial V/\partial N_i) dp - \ln(P/P_0) \quad (12)$$

Where ϕ_i^0 is the fugacity coefficient at pressure P_0 . Mathematical manipulation of term of the right hand side gives:

$$\ln(\phi_i/\phi_i^0) = \int_V^{V_0} (1/RT)(P/N_i) dv - \ln(Z/Z_0) + \ln(V_0/V) \quad (13)$$

Where Z = is the compressibility factor.

$$Z = (PV/nRT).$$

V_0 = the volume at pressure P_0 .

As V_0 become large, the behavior at V_0 will approach that of an ideal gas, so it is assumed that $\phi_i = 1$ and $Z_0 = 1$ then:

$$\ln \phi_i = \int_V^{\infty} [(1/RT)(\partial P/\partial N_i) - (1/V)] dv - \ln Z \quad (14)$$

This equation can be applied to either liquid or vapor phases and is used for driving fugacities from an equation of state.

Present Modeling Technique for V.L.E

The concept of vapor liquid equilibrium discussed above is applied here to multi-component hydrocarbon fluids in order to perform phase behavior calculations and simulate multi-contact miscibility and laboratory P. V. T. processes. The model is named "MIS-MODEL" that uses both M.S.R.K. and P. R. equations of state.

The solution technique used to solve the non-linear differential equations describing V. L. E. problem is successive iterative with aid of Aitken's method (where required close to critical region).

The model has four parts of calculations, these are:

1. C. M. and M. M. P.
2. Double point calculations.
3. Dew point calculations.
4. Other applications of phase behavior as:
 - PVT analysis for liquid and gas phases.
 - Pseudoization of C_n^+ .

The model can deal with hydrocarbon component and non-hydrocarbon components such as N_2 , CO_2 , H_2S .

Validation of "MIS-Model"

MIS model was tested by ten-runs with data from the literature in order to examine the validity of the results obtained and compare it with the original published values.

It was necessary that the choosed cases contain all the information (input data) required by the program. Statistical test such as standard deviation and absolute average percentage error were applied, the results obtained are summarized in Table 1 below:

Table (1)

No.	Actual MMP (Psi)	Predicted MMP (Psi)
A pool ⁽⁴⁾	5497	5500
D pool ⁽⁴⁾	5670	5600
E pool ⁽⁴⁾	6092	5750
Glaso-1 ⁽⁵⁾	5700	5750
Glaso-2 ⁽⁵⁾	6900	6900
Glaso-3 ⁽⁵⁾	5200	5200
Oil-A ⁽⁶⁾	4800	4950
Oil-B ⁽⁶⁾	5800	5600
Oil-C ⁽⁶⁾	6000	6000
Oil-D ⁽⁶⁾	6300	6350

S. D.-2.210% A. A. P. E 1.1730

Tuning of "MIS Model"

In order to make "MIS MODEL" more sensitive to the composition of Jambour cretaceous reservoir fluid, a tuning process was carried out by searching for the interaction coefficients that make the results in good agreement with pressure or saturation pressure at certain temperature.

For system involving examination of hydrocarbon phase behavior under injection/displacement condition it is required that the equation of state be able to cope with mixtures having a very high content of n-hydrocarbons (N_2 , CO_2 , H_2S). This means that testing of the equation

inadequacy requires the binary iteration coefficients for both hydrocarbon-hydrocarbon and hydrocarbon-non-hydrocarbon since they are the most influential variables.

The Jambour-Cretaceous miscibility study ⁽⁷⁾ shows that the reservoir fluid taken from the well Ja-27 with saturation pressure (4452 Psi) is a representative sample for the Jambour reservoir fluid, and its composition under saturation pressure was measured chromatographically and mentioned in Table (2). This can be considered as a base for the tuning of our model to the Jambour-Cretaceous reservoir fluid.

Tuning of Modified-Soave Redlich Kwong Equation of State

This study used the modified version of R. W- EOS by "Graboski and Doubert" ^(8,9) in (1978) for predicting phase behavior of hydrocarbon mixture. Through their investigation the interaction coefficients were correlated with solubility parameters to provide a general method for their estimation. The generalized coefficients are shown to produce the binary equilibrium data set accurately.

By incorporation of (Ja-27) reservoir fluid composition, under saturation pressure (4452 Psi) and reservoir temperature 210 °F with MIS-MODEL procedure two-an optimum convergence of MSRK-E. O. S. is obtained with the above coefficients. Figure (1) explains the behavior of the cubic equation according to the convergence criteria used and Tables (3, 4) give the values of the interaction coefficients.

Tuning of Peng Robinson Equation of State

Reservoir fluid composition under saturation pressure (4452 Psi) and reservoir temperature (210 °F) was also incorporated to the interaction coefficients ($C_{ij} = 0$) with PR-E.O.S. The first trial was made with ($C_{ij} = 0$) and the behavior of PR-E. O. S. is shown in Figure (2), the trend of the convergence for this cubic E. O. S. was normal but the stability of the equation behavior after (16-iteration) was less than the convergence criteria of (1×10^5), therefore other trials were under taken with other values for the interaction coefficients for the cubic equation according to their definitions. Through running the computer program it is observed that some of the interaction coefficient values cause the cubic equation to behave as monotonic wave and never reaches

convergence's. Also the behavior was very far from the convergence criteria. Figs. (3, 4) show this behavior.

In most computer models the interaction coefficients are set to be constant which was also followed in the above trial. However, Varotsis, et al ⁽¹⁰⁾ (1986) observed that those coefficients vary with temperature and pressure and they generalized a function for (CH_4 , N_2 , CO_2 -hydrocarbon) binaries and assumed these coefficient as a function of pressure, temperature and eccentric factor.

Therefore when using PR-EOS, Varotsis et al ⁽¹⁰⁾ procedure to calculate interaction coefficients is applied in order to tune the equation for Jambour-fluids. The results obtained in this case were partially different from the other runs. But in fact still very far from convergence this means that Varotsis equation does not work with our composition under reservoir temperature and saturation pressure.

The tuning process was continued in the trial and error procedure used earlier in order to get the correct values of (C_{ij}) and the optimum conditions of convergence. As a result the correct values were obtained, Tables (3) and (4) give the values of (C_{ij}) obtained and Fig. (5) show the optimum behavior of PR-EOS with Jambour cretaceous reservoir temperature 210 °F. Table (5) shows the composition of reservoir fluid predicted by MIS-MODEL, using values of C_{ij} from both Tables (3) and (4).

RESULTS AND DISCUSSION

In this study two equations of state are tuned for reservoir oil of Jambour field. Each equation was investigated in liquid and gas in order to determine which of them is more suitable for that phase.

Liquid Phase (Reservoir Oil at 210°F)

Results obtained from (MIS-MODEL) in running (MSRK and PR-EOS) with oil reservoir at 210 °F with wide range of pressure lead to the conclusion that the behavior of both equations is similar. With slight deviation in the result in low pressure region while there is convergence at high pressure region, this agree with the logical

formation of these equations, (MSRK-EOS) was found to be more suitable for liquid for liquid density determination than (PR-EOS), this phenomenon was also noted by Varotsis et al (97). They noticed a deviation +10% when applying (PR-EOS) in their model incorporating North Sea reservoir oil.

Gas Phase (Gas Cap at 210 °F)

Results obtained from (MIS-MODEL) using (MRSK and PR-EOS) incorporating gas cap at 210 °F with a range of pressure lead to the conclusion that the behavior of both equations is similar in comparison with experimental.

CONCLUSIONS

1. Optimum convergence of MRSK-F.O.S. was obtained when incorporating (Ja-27) reservoir fluid composition under saturation pressure (4452 Psi) and reservoir temperature 210 °F with interaction coefficient that were proposed by Graboski M. Daubert T. W. ^(8,9).
2. Very poor convergence was obtained when using the generalized interaction coefficient equation for PR-E.O.S. developed by Varotsis et al ⁽¹⁰⁾ in the tuning of the PR-E.O.S. for Jambour Cretaceous oil reservoir.
3. Now values of C_{ij} are obtained for tuning PR-E.O.S. with (Ja-27) Jambour Cretaceous oil reservoir and an optimum behavior of the cubic E.O.S. is noticed accordingly.
4. MRSK-E.O.S. gave a better performance than PR-E.O.S. for both liquid and gas phases.

NOMENCLATURE

C_{ij}	Interaction coefficient
F_i	Fugacity of component i
G	Gibbs free energy
H	Enthalpy
P	Pressure (Psi)
R	Gas constant (Psi*ft ³ /(lb. Mol) R°)
S	Entropy
T	Absolute temperature
V	Volume (ft ³ /lb. Mole)
X_i	Mole fraction of component i in liquid phase
Y_i	Mole fraction of component i in vapor phase
Z	Composition (mole fraction)
ϕ_i	Fugacity coefficient of component i

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Table (2) Reservoir Oil Composition Analysis from Well (Ja-27) by P.R.C

Component	Reservoir Pressure				
	4452 Psi	3982 Psi	3556 Psi	2987 Psi	2418 Psi
N ₂	0.149	0.135	0.122	0.129	0.127
CO ₂	3.092	2.991	2.956	2.883	2.801
H ₂ S	9.88	9.799	9.872	10.129	10.372
C ₁	60.751	58.281	55.236	50.548	45.361
C ₂	6.167	6.005	5.989	5.953	5.921
C ₃	2.201	2.091	2.139	2.145	2.239
iC ₄	0.273	9.253	0.248	0.245	0.259
nC ₄	0.744	0.688	0.678	0.667	0.674
iC ₅	0.230	0.205	0.198	0.192	0.190
nC ₅	0.283	0.25	0.278	0.227	0.228
C ₆	0.316	0.245	0.216	0.208	0.197
C ₇ ⁺	15.915	19.056	22.120	26.675	31.638

Table (3) Interaction Coefficient (C_{ij}-2) for PR-E.O.S

	N ₂	CO ₂	H ₂ S	C ₁	C ₂	C ₃	iC ₄	nC ₄	iC ₅	nC ₅	C ₆	C ₇ ⁺
N ₂	0	0										
CO ₂	0	0										
H ₂ S	0	0	0									
C ₁	0.12	0.15	0	0								
C ₂	0.12	0.15	0	0	0							
C ₃	0.12	0.15	0	0	0	0						
iC ₄	0.12	0.15	0	0	0	0	0					
nC ₄	0.12	0.15	0	0	0	0	0	0				
iC ₅	0.12	0.15	0	0	0	0	0	0	0			
nC ₅	0.12	0.15	0	0	0	0	0	0	0	0		
C ₆	0.12	0.15	0	0.025	0.01	0.01	0	0	0	0	0	
C ₇ ⁺	0.12	0.15	0	0.04	0.01	0.01	0	0	0	0	0	0

Table (4) Interaction Coefficient (C_{ij} -2) for PR-E.O.S

	N ₂	CO ₂	H ₂ S	C ₁	C ₂	C ₃	iC ₄	nC ₄	iC ₅	nC ₅	C ₆	C ₇ ⁺
N ₂	0											
CO ₂	-0.012	0										
H ₂ S	0.178	0.96	0									
C ₁	0.031	0.098	0	0								
C ₂	0.042	0	0	0	0							
C ₃	0.091	0.124	0	0.017	0	0						
iC ₄	0	0.131	0.049	0.03	-0.025	-0.008	0					
nC ₄	0	0.135	0.049	0.027	0.01	0.003	-0.002	0				
iC ₅	0	0.127	0	0	0	0	0.012	0	0			
nC ₅	0	0.127	0	0.029	0.009	0.028	0	0.017	0	0		
C ₆	0.149	0.149	0.11	0	0.04	-0.04	-0.001	-0.007	0	0	0	
C ₇ ⁺	0	0	0	0.037	0.007	0.007	0.007	0.004	0.01	0.01	-0.009	0

Table (5)

Component	x_i	Zx_i
<i>Nitrogen</i>		
Carbon dioxide	0.14	0.149
Hydrogen sulfide	3.09	3.092
Methane	9.88	9.88
Ethane	60.68	60.751
Propane	6.16	6.167
i-Butane	2.2	2.201
n-Butane	0.27	0.273
i-Pentane	0.74	0.744
n-Pentane	0.23	0.23
Hexane	0.28	0.283
Heptane plus	0.31	0.316
	15.96	15.915

Bubble point pressure = 4452 psi, using $C_{ij} = 1$, No. of iteration = 19, moles of liquid = 1, convergence factor for bubble point pressure: $G = 1$

Component	x_i	Zx_i
<i>Nitrogen</i>		
Carbon dioxide	0.14	0.149
Hydrogen sulfide	3.09	3.092
Methane	9.88	9.88
Ethane	60.68	60.751
Propane	6.16	6.167
i-Butane	2.2	2.201
n-Butane	0.27	0.273
i-Pentane	0.74	0.744
n-Pentane	0.23	0.23
Hexane	0.28	0.283
Heptane plus	0.31	0.316
	15.96	15.915

Bubble point pressure = 4452 psi, using $C_{ij} = 2$, No. of iteration = 20, moles of liquid = 1, convergence factor for bubble point pressure: $G = 0.99997$

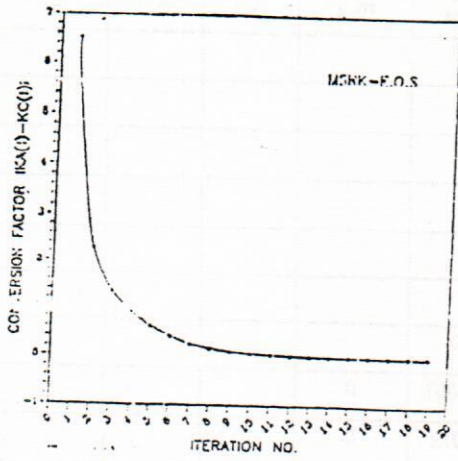


Fig. (1)

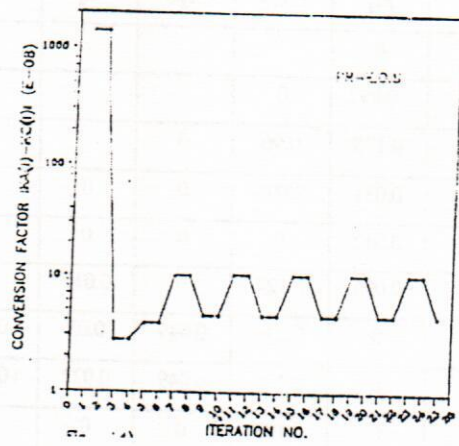


Fig. (4)

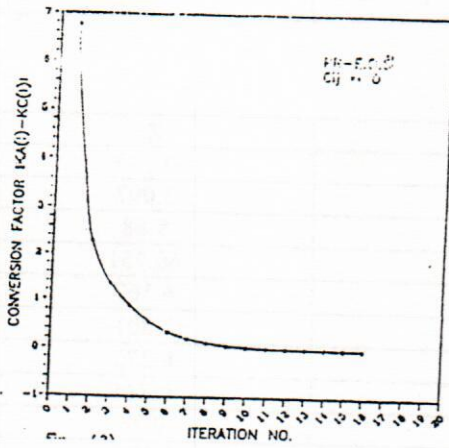


Fig. (2)

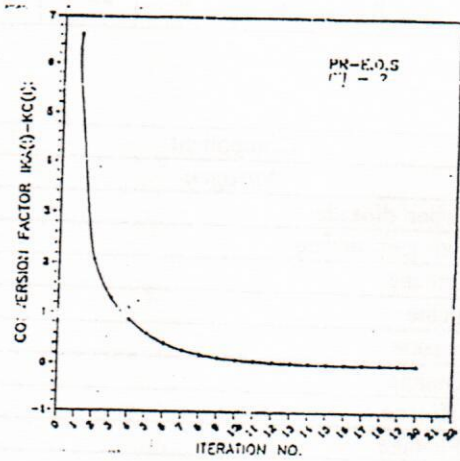


Fig. (5)

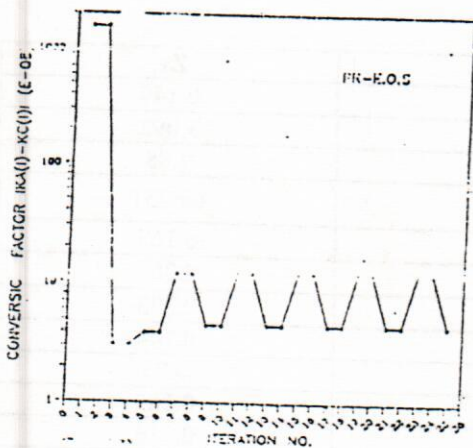


Fig. (3)