Reduction of Reservoir Fluid Equilibrium Calculation for Peng-Robinson EOS with Zero Interaction Coefficients

Mahdi Assareh*

Thermodynamics Research Laboratory, School of Chemical Engineering, Iran University of Science and Technology, Tehran, Iran

ABSTRACT

For some of the EOS models the dimension of equilibrium problem can be reduced. Stability and difficulties in implementation are among the problems of flash calculation. In this work, a new reduction technique is presented to prepare a reduced number of equilibrium equations. Afterwards, a number of appropriate solution variables are selected for the prepared equation system to solve the equations in an efficient numerical scheme. All the derivatives and solution procedures for the new reduced flash calculation framework were prepared based on Peng-Robinson equation of state. One reservoir oil sample and one gas condensate sample were selected from published literature to evaluate the proposed method for the calculations of reservoir fluids equilibrium. The equilibrium calculations with the proposed reduction technique were compared to full flash calculations. The reduced formulation implementation is simple and straightforward as it is derived from full flash fugacity equality criteria. The presented technique not only reduces the number of equations, and hence simplifies flash problem, but also presents a comparable convergence behavior and offers the same solution system for different reservoir fluid types. The results, demonstrates the proposed method performance and the accuracy for modeling with complex equilibrium calculations like compositional reservoir simulation when there are many components available in the mixture fluid description.

Keywords: Reduction, Flash calculation, Reservoir Fluids, Peng-Robinson, Cubic Equation of States

INTRODUCTION

Stability analysis and equilibrium calculations are repeated several times for many reservoir simulation cells for the field studies with compositional reservoir simulation using equations of state (EOS). It is shown that that equilibrium calculation is an important part of the CPU time, depending discretization, non-linearity, process complexity and degree of implicitness [1].

For EOS models, the dimensionality of equilibrium problem can be reduced. Originally reduction techniques were introduced for the mixtures in which all the binary interaction coefficients are zero. Michelsen (1986) found that the dimensionality of the flash calculation by cubic EOS with zero interaction coefficients is three [2]. He explained that zero binary interaction coefficients permit very significant simplifications in the calculation of phase equilibrium for multicomponent mixtures, in particular when the

number of components is high. He proposed to solve three equations with three unknowns to find the equilibrium ratios. This means that the dimensionality of the two phase flash problem is independent of the number of components for cubic EOS. He mentioned that each component having non-zero interaction coefficients with the other components introduces two new equations in case that the added binary interaction coefficient (BIC) is between two components other than previous BIC's component. Two BIC's with one common component add 3 more equations. Michelsen selected three errors (equations) to solve for final equilibrium composition for each phase. In Michelsen method, an initial estimation of the reduced flash variables is used to start calculations. Assuming zero binary interaction coefficients, n_v (the number of moles in vapor phase), a_v and b_v are selected as variables ($\zeta=[n_v, a_v, b_v]^T$):

$$a_v=\sum_{i=1}^{nc}\sum_{j=1}^{nc} y_i y_j (a_j a_j)^{1/2}=(\sum_{i=1}^{nc} y_j (a_j)^{1/2})^2=(\alpha_v)^2 \quad (1)$$

$$b_v=\sum_1^{nc} y_j b_j \quad (2)$$

The liquid phase parameters can be calculated based on vapor phase parameters and feed parameters:

$$\alpha_l=(\alpha_f - n_v \alpha_v)/(1-n_v) \quad (3)$$

$$b_l=(b_f - n_v b_v)/(1-n_v) \quad (4)$$

Michelsen selected three errors (following equations) to solve for final equilibrium composition of each phase $(g=[g_1, g_2, g_3]^T)$:

$$g_1=\sum_1^{nc}(u_j^l - u_j^v) \quad (5)$$

$$g_2=\sum_1^{nc} u_j^v \alpha_{iv} - \alpha_v \quad (6)$$

$$g_3=\sum_1^{nc} u_j^v b_{iv} - b_v \quad (7)$$

In Michelsen method, an initial estimation of reduced flash variables is used to start calculations. Based on these variables and with the help of

Equations 3 and 4, the fugacity coefficients are calculated to update liquid and vapor composition, namely u_j^v and u_j^l. The new compositions are used to solve the reduced equations. The reduced variables are updated after solution and this cycle is repeated until convergence is obtained. However, for gas condensate systems, it is recommended that the corresponding variables be selected for the liquid phase. This recommendation comes from different sets of equations and different variables selection. It should be emphasized that all of these equations are in fact different versions of the equality of chemical potential equations; therefore, if it is possible to have an analytical solution for the flash calculation problem, the solution must then be the same. But since the flash calculation problems are solved numerically, the selection of the equations and solution variables and numerical scheme for it can affect the final calculation results. Based on these variables, the fugacity coefficients are calculated to update liquid and vapor composition.

Jensen and Fredenslund (1987) extended the Michelsen method for the situations where one non-zero interaction coefficient exists in the mixture by solving a system of only five equations [3]. They assumed one BIC for non-hydrocarbon–hydrocarbon interactions. As previously discussed, the non-zero BIC brings two equations in addition to 3 existing equations. This procedure is advantageous for CO_2 and nitrogen flooding in the reservoirs. To solve the equations, they selected five variables.

The variables in the flash problem are vapor mole fraction, n_v, and first component (non-hydrocarbon component) mole fraction as well as:

$$al_v=\sum_2^{nc} y_j a_j^{1/2} \quad (8)$$

$$dl_v=\sum_2^{nc} y_j a_j^{1/2} Kij \quad (9)$$

$$gl_v=\sum_2^{nc} y_j b_j \quad (10)$$

With these variables, the attraction and repulsion terms for gas phase can be calculated as:

$$a_v = x_1^2 a_1 + 2x_1 a_1^{1/2} (al_v - dl_v) + al_v^2 \qquad (11)$$

$$b_v = x_1 b_1 + gl_v \qquad (12)$$

In this relations, x_1 and y_1 are the mole fraction of the first component (non-hydrocarbon component). The following equations are used to calculate corresponding parameters for liquid phase:

$$al_l = (al_f - n_v al_v)/(1 - n_v) \qquad (13)$$

$$dl_l = (dl_f - n_v dl_v)/(1 - n_v) \qquad (14)$$

$$gl_l = (gl_f - n_v gl_v)/(1 - n_v) \qquad (15)$$

$$x_1 = (z_1 - y_1 n_v)/(1 - n_v) \qquad (16)$$

where, al_v, dl_v, gl_v, y_1, and n_v are taken as the solution variables ($\zeta = [n_v, al_v, dl_v, gl_v, y_1]^T$). An initial guess is used to start reduced flash procedure. The corresponding liquid phase parameters are computed according to Equations 13-16. Afterwards, the liquid and vapor compositions are calculated with fugacity equations using above variables. Jensen and Fredenslund used the following set of equations to be solved for the five variables ($g = [g_1, g_2, g_3, g_4, g_5]^T$):

$$g_1 = \sum_2^{nc} u_j a_j^{1/2} - al_v \qquad (17)$$

$$g_2 = \sum_2^{nc} u_j a_j^{1/2} K_{1i} - dl_v \qquad (18)$$

$$g_3 = \sum_2^{nc} u_j b_j - gl_v \qquad (19)$$

$$g_4 = u_1 - y_1 \qquad (20)$$

$$g_5 = \sum_{j=1}^{N} u_j - y_j \qquad (21)$$

The updated five variables after equation solution are then used to calculate the liquid and gas composition and the loop is repeated until the convergence. Therefore, again one of the drawbacks of Jessen and Fredenslund method is the different sets of equations relative to full equilibrium equations. This causes different solution behaviors

for different thermodynamic conditions and reservoir fluid types relative to full flash approach as it is described in Michelsen technique.

Hendriks (1988) presented a general mathematical theorem in phase equilibrium equations to show how for a well-defined class of thermodynamic models (e.g. cubic EOS) the dimensionality of various phase equilibrium problems can be reduced [4].

Li and Johns developed an effective method for reduced flash calculation in cases that non-zero interaction coefficients are existing in the fluid description [5]. They presented a new method to increase the speed of flash calculations for any numbers of nonzero BIP's. The approach requires the solution of up to six reduced parameters regardless of the number of components and is based on decomposing the BIP's into two parameters using a simple quadratic expression. The new approach is exact in that the equilibrium-phase compositions for the same BIP's are identical to those with the conventional flash calculation; no eigenvalue analysis is required. However, the calculated equilibrium ratios are estimations of full flash equilibrium ratios. The drawback of such approach is that the equilibrium ratios are the estimation of full flash equilibrium ratio. Different applications of the reduction methods have been investigated by Nichita et al. to prove their exactness for a wide range of equilibrium calculation problems such as stability analysis, saturation pressure, extrapolation of the results of previously performed flashes with different application from synthetic hydrocarbon to real petroleum reservoir mixtures, and multiphase flash calculations [6].

Hoteit and Firoozabadi (2006) presented an algorithm for the stability analysis in the reduction method. In their technique, the Newton method is used in the solution of nonlinear equations except in some isolated iterations when one single successive

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substitution iteration may be required to avoid nonphysical conditions [7].

Nichita and Graciaa (2011) developed a general workflow for flash calculation with reduction techniques for cubic EOS in cases that there are more than one non-zero interaction coefficients [8]. Also, comparisons of the proposed numerical schemes for reduction techniques are available in the literature [9].

They described that, in a classical reduction method for phase equilibrium calculations, there are M reduction parameters, $Q_p=(Q_{p1},Q_{p2},…,Q_{pM})^T$:

$$Q_p= \sum_{i=1}^{nc} q_{\alpha i} x_{ip}, \ \alpha =1, M, p=L \ or \ V \qquad (22)$$

The M+1 error equations are given by:

$$e_\alpha= \sum_{i=1}^{nc} q_{\alpha i} x_{ip}- Q_{p\alpha}, \ \alpha=1, M, p=L \ or \ V \qquad (23)$$

$$e_{M+1}= \sum_{i=1}^{nc} (y_i- x_i) = 0 \qquad (24)$$

choice between these two is made depending on which phase is the least abundant.

Gaganis et al. (2012) presented a general framework for developing solutions to Rachford-Rice equation utilizing function classes, the members of which exhibit a behavior similar to that of the equation to be solved. Fitting such functions, instead of a simple straight line at each iteration of the solution process, as is the case of the Newton–Raphson approach, leads to better subsequent estimates and thus to faster convergence [10]. In this approach, the calculated equilibrium ratios with the reduced technique are the estimation of full flash equilibrium ratios.

Gaganis and Varotsis (2013) replaced the conventional spectral decomposition [8] using basis vectors by new ones so that the approximation error of the energy parameter is minimized. The new reduced variables set leads to improved flash calculations accuracy, thereby allowing them to be performed at a given accuracy level using fewer reduced variables compared to the

conventional approach [11].

Gorucu and Johns (2014) presented new reduced parameters using the two-parameter binary interaction parameter formula originally proposed by Li and Johns (2006) [12]. The new reduced parameters were employed to solve two-phase flash calculations for five different fluid descriptions. Later on, an applied phase-related equilibrium (APPLE) solver using only the Peng–Robinson equation of state was developed based on rigorous classical thermodynamics [13] with a theoretically and thermodynamically consistent solver with the stringent equilibrium criterion.

Gaganis and Varotsis (2014) presented an integrated approach to provide direct answers to both the phase stability and phase split problems during compositional modeling using a regression approach. The non-linear transformation of the equilibrium equations is combined to explicit expressions, which are generated to provide directly the solution of the phase-split problem within the reduced variables. Regression models are developed so as to estimate pressure and temperature to the prevailing values of the reduced variables set with a direct function relating feed composition [14].

Petitfrere and Nichita (2015) provided an improvement of two-phase reduced flash calculations [15] to multiphase equilibrium calculation with any number of phases. They proposed their algorithms with two approaches, a direct extension of the reduction for two-phase flashes and a Gibbs free energy constrained minimization. They examined their proposed algorithms for several multiphase systems containing hydrocarbon components, carbon dioxide, and hydrogen sulfide. Numerical experiments showed that the reduction methods for multiphase flash calculations become faster than the conventional methods when the number of components increases,

when the number of equilibrium phases increases, and when the number of BIC decreases. They claimed that for samples with many components and few BIC's, their method can improve the equilibrium calculation performance [16].

Petitfrere and Nichita (2015) evaluated stability testing and flash calculations separately. It is shown that reduction methods are more efficient than conventional techniques, so they are suitable for compositional simulation. This is beneficial specially because, in most of the reservoir simulators, no explicit phase split is required and equilibrium calculations are parts of a larger problem (coupled with flow equations), while phase stability analysis must be performed in most grid blocks [17].

The non-linear nature of phase equilibrium calculations requires an iterative solution procedure. Stability and difficulties in implementation are among the problems with flash calculation reduction [18]. In this work, a new reduction technique is presented. In this respect, a reduced number of equilibrium equations was prepared. Afterwards, appropriate solution variables are selected for the prepared equations system to solve the equations in an efficient numerical scheme. All the derivatives and solution procedures for the new reduced flash calculation framework were prepared based on Peng-Robinson equation of state. The proposed approach has two advantages over conventional reduction technique. The first is the unique set of equations and variables for different types of the reservoir fluids. Secondly, having the same equations and the same variables ensures that the convergence behavior of the reduced flash numerical scheme is the same as full flash scheme, and there is no need to change the equation systems and solution variables. Besides, the numerical scheme thresholds can be provided directly from the full flash approach. The other advantage of the reduction

technique is that the formulations are just extracted from the full flash algorithms; therefore, there is no considerable difficulties regarding implementation.

Reservoir Fluid Samples

Three main hydrocarbon groups, namely paraffins, naphthenes, and aromatics, are usually available in any petroleum reservoir fluid mixtures. Paraffins are divided into two groups of normal-paraffins and iso-paraffins. Naphthenes or cycloalkanes are rings or cyclic saturated hydrocarbons. Cyclo-pentane, cyclohexane, and their derivatives are normally found in crude oils. The content of naphthenes in petroleum may vary up to 60% [19]. Aromatics are an important series of hydrocarbons found in almost every petroleum mixture from any area of the world. Usually a sample of petroleum fluid is characterized as discrete components, petroleum cuts, and a plus fraction. Each fraction contains paraffinic, naphthenic, and aromatic components. Usually the fractions molecular weight, specific gravity, and normal boiling point are measured and reported. Specific gravity (S) and molecular weight (MW) are useful parameters for the characterization of petroleum fluids to determine PNA composition and also to estimate other properties such as critical constants, density at various temperatures, viscosity etc. In this work, the new reduction technique on equilibrium calculations is examined for two samples of reservoir fluid. Sample 1 (S1) is an oil reservoir fluid characterized with 24 components. Samples S1 data were taken from published data [20]. The sample characterization data are presented in Table 1. The data for sample 2 is obtained from North Sea gas condensate by Leibovici et al. (1993) including 27 components [6]. The characterization data are reported in Table 2 for this sample

Table 1: S1, Fluid Characterization

Components	ZI (percent)	MW	P_c (bar)	T_c (K)	AF	V_c (m³/kg.mol)
N_2	0.1800	28.0130	33.9440	126.2000	0.0400	0.0900
CO_2	0.8200	44.0100	73.8660	304.7000	0.2250	0.0940
C_1	22.9200	16.0430	46.0420	190.6000	0.0130	0.0980
C_2	7.2100	30.0700	48.8390	305.4300	0.0986	0.1480
C_3	7.3700	44.0970	42.4550	369.8000	0.1524	0.2000
IC_4	1.5800	58.1240	36.4770	408.1000	0.1848	0.2630
nC_4	5.2300	58.1240	37.9660	425.2000	0.2010	0.2550
IC_5	2.2500	72.1510	33.8930	460.4000	0.2270	0.3080
nC_5	3.6000	72.1510	33.7010	469.6000	0.2510	0.3110
C_6	4.8400	86.0000	31.7970	500.4300	0.2675	0.3551
C_7	4.7200	92.0000	31.8080	523.8600	0.2913	0.3721
C_8	4.5200	102.0000	30.4830	552.2700	0.3254	0.4068
C_9	4.0700	117.0000	28.1190	586.8300	0.3752	0.4623
C_{10}	3.5000	134.0000	25.5580	619.6700	0.4315	0.5271
C_{11}	2.9100	151.0000	22.7690	642.7500	0.4898	0.5977
C_{12}	2.4200	165.0000	21.0210	662.6900	0.5370	0.6539
C_{13}	1.9900	178.0000	19.6780	681.2900	0.5801	0.7050
C_{14}	1.7400	194.0000	18.2980	704.1200	0.6323	0.7666
C_{15}	2.0200	208.0000	17.4260	726.2000	0.6757	0.8174
C_{16}	1.3900	225.0000	15.9750	743.9100	0.7322	0.8871
C_{17}	1.2100	239.0000	14.9500	758.4800	0.7780	0.9439
C_{18}	0.9000	249.0000	14.3960	770.6900	0.8092	0.9820
C_{19}	1.1700	270.0000	13.2320	793.3500	0.8754	1.0643
C_{20+}	11.4400	560.0000	4.9241	1021.2000	1.5499	2.2181

Table 2: S2 fluid characterization

Components	ZI (percent)	T_c (K)	P_c (Bar)	AF	MW
N_2	0.3243	126.2000	33.9400	0.0400	28.0100
CO_2	1.9549	304.2000	73.7700	0.2250	44.0100
C_1	76.1530	190.6000	46.0000	0.0115	16.0400
C_2	7.7367	305.4000	48.8400	0.0908	30.0700
C_3	3.6177	369.8000	42.4500	0.1454	44.1000
iC_4	0.5667	408.1000	36.4800	0.1760	58.1200
nC_4	1.3258	425.2000	38.0000	0.1928	58.1200
iC_5	0.4480	460.2600	33.8300	0.2271	72.1500
nC_5	0.6100	469.6000	33.7400	0.2273	72.1500
CC_5	0.0580	511.6000	45.0900	0.1923	70.1400
PC_6	0.6001	503.7900	30.0700	0.2860	86.1800
CC_6	0.4148	547.4100	39.9000	0.2215	84.1600
AC_6	0.1735	562.1000	48.9400	0.2100	78.1100
PC_7	0.4239	536.4400	27.6000	0.3364	100.2100
CC_7	0.5056	566.2700	34.6900	0.2451	98.1900
AC_7	0.3063	591.7000	41.1400	0.2566	92.1400
PC_8	0.3291	565.0500	25.0200	0.3816	114.2300
CC_8	0.2540	594.0500	29.7400	0.2391	112.2100
AC_8	0.2564	619.4600	35.8400	0.3228	106.1600
PC_9	0.2630	590.6400	23.2900	0.4230	128.2500
CC_9	0.1640	621.2100	28.3900	0.2998	125.9700
AC_9	0.1217	644.0600	32.0800	0.3725	120.1600
PC_{10}	0.2411	613.7200	21.4600	0.4646	142.2800
CC_{10}	0.0427	621.5800	26.2500	0.4058	140.2000
AC_{10}	0.1049	670.8300	29.7200	0.3642	133.8000
CN_{-1}	2.6703	711.0400	18.7500	0.8000	240.0000
CN_{-2}	0.3338	848.0800	16.3300	1.3000	450.2600

Reduction Technique

For a two phase flash calculation problem, the following system of nonlinear equations is solved:

$$g_i = \ln K_i + \ln \varphi_i^v (y,P,T) - \ln \varphi_i^l (x,P,T) = 0 \quad i=1,...,n_f \quad (25)$$

where, φ_i denotes the fugacity coefficient of component i calculated using EOS. To calculate the fugacity coefficients for each phase p, one should recall PR EOS. If we define the following constants:

$$p_1 = -2\sqrt{2}, \ p_2 = 1 - \sqrt{2}, \ p_3 = 1 + \sqrt{2} \quad (26)$$

Compressibility factor is calculated based on PR EOS as for each phase p:

$$Z_P^3 - (1 - B_P)Z_P^2 + (A_P - 2B_P - 3B_P^2)Z_P$$
$$-(B_P A_P - B_P^2 - B_P^3) = 0 \quad (27)$$

In this cubic equation of state, capital EOS parameters, A_p and B_p) are calculated according to small EOS parameters, a_p and b_p:

$$A_p = \frac{a_p}{(RT)^2}, \ B_p = \frac{b_p}{(RT)^2} \quad (28)$$

The small EOS parameters are resulted from *VdW* mixing rules, if the binary interaction coefficients are zero

$$a_p = \sum_{i=1}^{nf}\sum_{j=1}^{nf} x_{pi} x_{pj} \sqrt{a_i a_j} \ , \ b_p = \sum_{i=1}^{nf} x_{pi} b_i \quad (29)$$

If binary interaction coefficients are not zero, the outcome of the reduced flash problem can be used as an initial estimate of the full flash problem. This makes advantages when we are dealing with near critical fluid with lots of components in the mixture. Moreover, usually the petroleum reservoir fluids contain non-well-defined fractions and plus fractions. The critical and thermos-physical properties of such fractions are estimated through correlations and readjusted through tuning procedures. That is why there are cases in which the petroleum engineers prefer to tune these estimated properties instead of binary interaction coefficients to match saturation pressure and PVT experiments. The fugacity coefficients for phase p for each component are given by:

$$Ln\varphi_i^P = \frac{b_i}{b^P}\left(Z^P - 1\right) - Ln\left(Z^P - B^P\right) -$$
$$\frac{A^P}{B^P P_1}\left(\frac{2s^P}{a^P} - \frac{b_i}{b^P}\right).Ln\left(\frac{Z^P + B^P p_2}{Z^P + B^P p_3}\right) \quad (30)$$

in which,

$$s^P = \sum_{j=1}^{nc} x^P_j a_j^{0.5} \quad (31)$$

The fugacity coefficients for each phase can be decomposed into three parts:

$$Ln\varphi_i^P = A_1 p + A_2^P b_i / bmix + A_3^P a_i^{0.5} \quad (32)$$

The coefficients, required for each component, are:

$$A_1^P = -Ln\left(Z^P - B^P\right) \quad (33)$$

$$A_2^P = bmix.(\frac{\left(Z^P - 1\right)}{b^P} + \frac{A^P}{B^P b^P p_1}Ln\left(\frac{Z^P + B^P p_2}{Z^P + B^P p_3}\right) \quad (34)$$

$$A_3^P = -\frac{A^P}{B^P p_1}\left(\frac{2s^P}{a^P}\right)Ln\left(\frac{Z^P + B^P p_2}{Z^P + B^P p_3}\right) \quad (35)$$

In this relation, *bmix* has a fixed value and calculated based on feed mole fractions:

$$bmix = \sum_{i=1}^{NC} z_i b_i \quad (36)$$

(This constant factor is added so that the magnitude of A_1^P, A_2^P, and A_3^P changes to the same order required for future calculation. By defining the below equations, one can easily calculate the equilibrium ratios (Equation 40):

$$\zeta_1 = A_1^L - A_1^V \quad (37)$$

$$\zeta_3 = A_3^L - A_3^V \quad (38)$$

$$\zeta_2 = A_2^L - A_2^V \quad (39)$$

$$\ln K_i = \zeta_1 + \zeta_2 . \frac{b_i}{bmix} + \zeta_3 . a_i^{0.5} \quad (40)$$

This equation provides the framework for the reduction technique. The liquid and vapor compositions are changing in each non-linear iteration of flash problem. Therefore, in each iteration, ζ_1, ζ_2, and ζ_3 are updated, and consequently the equilibrium ratios are updated; at the end of flash calculation, there is no more change in equilibrium ratios and in these parameters. Generally, in conventional flash calculation algorithms, the K-values in each iteration are updated with the following relation:
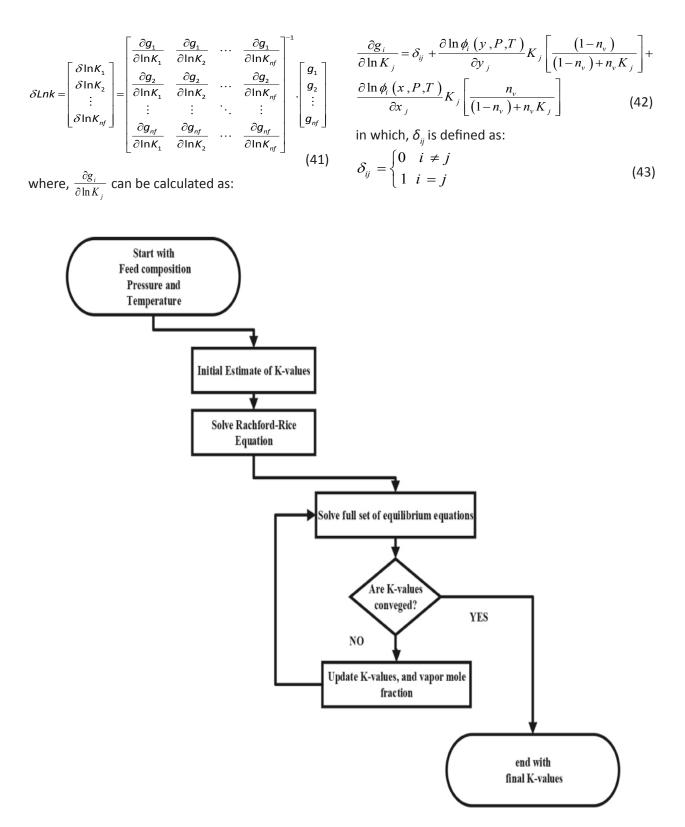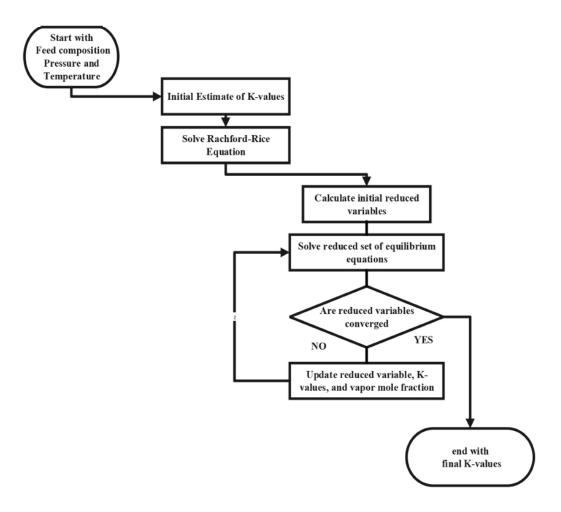
$$\delta Lnk = \begin{bmatrix} \delta \ln K_1 \\ \delta \ln K_2 \\ \vdots \\ \delta \ln K_{nf} \end{bmatrix} = \begin{bmatrix} \dfrac{\partial g_1}{\partial \ln K_1} & \dfrac{\partial g_1}{\partial \ln K_2} & \cdots & \dfrac{\partial g_1}{\partial \ln K_{nf}} \\ \dfrac{\partial g_2}{\partial \ln K_1} & \dfrac{\partial g_2}{\partial \ln K_2} & \cdots & \dfrac{\partial g_2}{\partial \ln K_{nf}} \\ \vdots & \vdots & \ddots & \vdots \\ \dfrac{\partial g_{nf}}{\partial \ln K_1} & \dfrac{\partial g_{nf}}{\partial \ln K_2} & \cdots & \dfrac{\partial g_{nf}}{\partial \ln K_{nf}} \end{bmatrix}^{-1} \cdot \begin{bmatrix} g_1 \\ g_2 \\ \vdots \\ g_{nf} \end{bmatrix}$$

(41)

where, $\dfrac{\partial g_i}{\partial \ln K_j}$ can be calculated as:

$$\frac{\partial g_i}{\partial \ln K_j} = \delta_{ij} + \frac{\partial \ln \phi_i (y,P,T)}{\partial y_j} K_j \left[\frac{(1-n_v)}{(1-n_v)+n_v K_j} \right] + \frac{\partial \ln \phi_i (x,P,T)}{\partial x_j} K_j \left[\frac{n_v}{(1-n_v)+n_v K_j} \right]$$

(42)

in which, δ_{ij} is defined as:

$$\delta_{ij} = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases}$$

(43)

Figure 1: Flowchart of the full flash as a basis for reduced flash.

Figure 2: Flowchart of the reduced flash.

For which, the required derivatives are derived in the appendix. It should be noted that the equilibrium equations and Rachford-Rice equation can be solved sequentially. This means that with a set of updated equilibrium ratios, the Rachford-Rice equation is solved, and the resulting mole numbers of vapor of the next set of equilibrium ratios are calculated. In this way, $n_v = 1-n_l$ can be regarded independent of equilibrium ratio in the internal loop for K-value updating. The work flow for the full flash calculation is presented in Figure 1.

The Rachford-Rice equation, a nonlinear equation, is solved for the molar fraction of each phases using Newton-Raphson method:

$$f\left(n_l\right) = \sum_{i=0}^{NC}\left(y_i - x_i\right) = \sum_{i=0}^{NC} z_i\left(k_i - 1\right)$$

$$/\left(n_l + \left(1 - n_l\right)k_i\right) = 0, \tag{44}$$

This equation is solved in an external loop. The solution to flash calculation problem is started with pressure, temperature, and feed composition. The initial estimate of K-Values is provided from Wilson correlation. The Rachford-Rice equation is solved iteratively until the mole number of vapor phase does not change anymore. With this in hand, the full set of equilibrium equations, as formulated in Equation 25, is solved based on a Newton approach for a set of non-linear solution using Equation 41. In the updating step, the difference in K-values is simply added to the K-values of the previous step. It should be mentioned that to update the mole number of vapor phase, there is no need to completely solve the Rachford-Rice in each iteration. One can use the following relation (with no need to iterate):

$$nv^{new} = nv^{old} - f(nv)/f'(nv) \qquad (45)$$

where, $f(nv)$ and $f'(nv)$ are calculated using Equations 44. Now if one considers Equation 40, all the equilibrium constants are functions of ζ_1, ζ_2, and ζ_3. ζ_1, ζ_2, and ζ_3 are the same for all of the mixture components. Therefore, one can set up the following set of variables:

$$\zeta_r^T = [\zeta_1, \zeta_2, \zeta_3]_{nr} \qquad (46)$$

In fact, if one could find the above vector, the K-values can be exactly calculated. Consequently, if there is no non-zero interaction coefficient, the problem dimensionality is 3. The proper reduced equilibrium equations to be solved for the reduced flash calculation are defined as:

$$g_r^T = \left[g_{IK(1)}, g_{IK(2)}, g_{IK(3)} \right]_{nr} \qquad (47)$$

where, IK returns the serial number of related equilibrium equation according to Equation 25. For components with zero interaction coefficients, the first three equations can be selected from three optional components. The solution of the reduced system is:

$$\delta\zeta_{nr} = [\delta\zeta_1, \delta\zeta_2, \delta\zeta_3]_{nr}^T = -J_{nr*nr}^{-1} \cdot g_{nr} \qquad (48)$$

To solve the reduced equation with the reduced number of variables, one needs to have the below relation for Jacobian calculation (J_{nr*nr} is extracted from J_{nf*nr}):

$$J_{nf*nr} = \left[\frac{\partial g}{\partial \zeta} \right]_{nf.nr} = \left[\frac{\partial g}{\partial Lnk} \right]_{nf.nf} \cdot \left[\frac{\partial Lnk}{\partial \zeta} \right]_{nf.nr} \qquad (49)$$

where, $[\partial g / \partial Lnk]_{nf.nf}$ is calculated from Equation 41. The second part of the calculation of these derivative, $[\partial Lnk / \partial \zeta]_{nf.nr}$, is in fact constant during flash iteration and is defined as the following relation:

$$\frac{\partial g_i}{\partial \zeta_1} = 1 \qquad (50)$$

$$\frac{\partial g_i}{\partial \zeta_2} = \frac{b_i}{bmix} \qquad (51)$$

$$\frac{\partial g_i}{\partial \zeta_3} = a_i^{0.5} \qquad (52)$$

The initial estimate of K-Values and the mole number of vapor phase are calculated based on Wilson and Rachford-Rice equation correspondingly. These values are then used as the basis for the initial estimation of the reduced variables. Afterwards, the reduced equation system in Equation 48 is solved to calculate the new reduced variables. These reduced set of variables are used to update the new full set of equilibrium ratio. The schematic diagram is shown in the Figure 2.
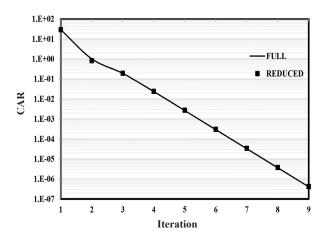

Figure 3: Convergence behavior of full flash calculation and the reduced technique for cumulative absolute residual (CAR); S1; P=50 bar; T= 550 K.
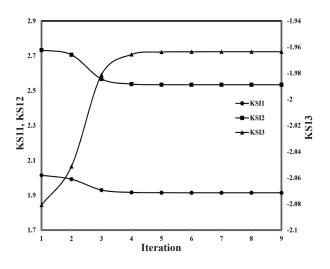

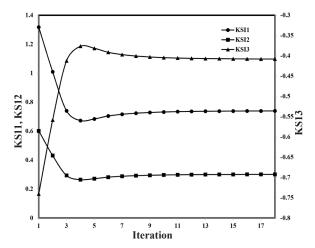**Figure 4: Variable changes during Newton-Raphson iteration; S1; P=50 bar; T= 550 K.**

Figure 5: Variable changes during Newton-Raphson iteration; S1; P=45 bar; T=900 K.

RESULTS AND DISCUSSION

To evaluate the proposed solution technique, two real reservoir samples, namely S1 and S2, were used. The initial equilibrium ratios were calculated with Wilson correlation.

$$K_i = \left(Pc_i / P\right).exp\left[5.37 \ \left(1 + \omega_i\right)\left(1 - Tc_i / T\right)\right] \quad (53)$$

Using these equilibrium ratios, the initial estimate of the reduced variable is calculated and the reduction flash calculation starts the mentioned numerical scheme. The convergence criteria for both flash types, i.e. the full flash and reduced calculations, are calculated based on:

$$\sum_1^{nf}\left|\ln K_i + \ln\varphi_i^v\left(y, P, T\right) - \ln\varphi_i^l\left(x, P, T\right)\right| < 10^{-6} \quad (54)$$

which is the cumulative absolute residual (CAR) and ensures the equality for the components in oil and gas phase due to the equilibrium conditions. The oil sample equilibrium reduction was tested in several pressures and temperatures inside a two phase region. At a pressure of 50 bar and a temperature of 550 K, the reduction results are presented. Figure 3 shows the close convergence behavior of the reduced and full flash approach. Both algorithms started from the same cumulative absolute residual due to the same initial estimates from Wilson equation.

The reduced variable changes during the Newton iterations are plotted in Figure 4. It shows that nearly after four or five nonlinear iterations, the reduced variables become very close to their final values. The same results but at a temperature of 900 K, where we have a little amount of oil, are plotted in Figure 5. The equilibrium ratios of the reduced approach are essentially the same as those shown in Figure 6.
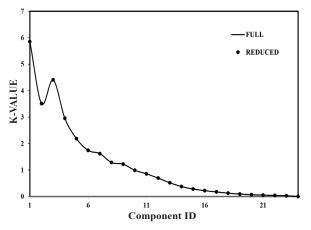

Figure 6: Equilibrium ratio comparison for the reduced and full flash calculation; S1; P= 50 bar; T= 550 K.

For the gas condensate sample, the equilibrium calculations at several pressures and temperatures inside the two phase region were performed. The convergence results are presented at 200 bar and 350 K. The decrease in the cumulative absolute residual during iterations in the full and reduced flash is plotted in Figure 7. The similar convergence behavior for both approaches is deduced from this figure. As it is expected for the gas condensate sample, the program needs a higher number of iterations to satisfy the equality of the fugacity coefficients in equilibrium. The changes in reduced variable during the Newton iterations in the conditions of 200 bar/350 K and 100 bar/300 K, where we have two completely different mole numbers of vapor phase, are plotted in Figure 8 and Figure 9 correspondingly. Here again, in both figures, the reduced variables become very close to their final values in less than five iterations.

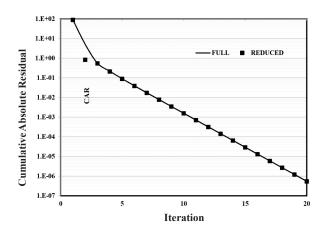The calculated reduced equilibrium ratios are plotted versus the full flash equilibrium ratios in Figure 10

Figure 7: Convergence behavior of full flash calculation and reduced technique for cumulative absolute residual (CAR); S2; P= 200 bar and T= 350 K.
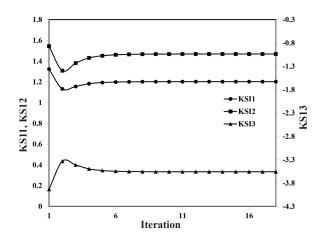

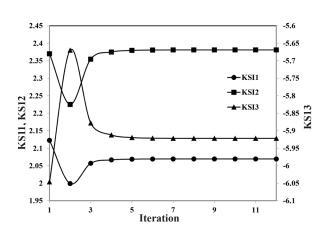**Figure 8: Variable changes during Newton-Raphson iteration; S2; P= 200 bar; T= 350 K.**

Figure 9: Variable changes during Newton-Raphson iteration; S2; P= 100 bar; T=300 K.
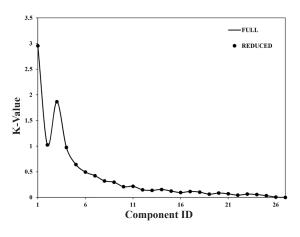

Figure 10: Equilibrium ratio comparison for the reduced and full flash calculation; S2; P=200 bar; T=350 K.

CONCLUSIONS

A new flash reduction technique is presented and verified against the full flash procedure. The proposed approach offers a unique set of equations and variables to reduce the dimension of the equilibrium calculation problem. In this method, the selection of the solution variables and reduced equations extend the stability and convergence of the proposed technique to support different reservoir fluid types and thermodynamic conditions. To demonstrate these capabilities, two real samples of reservoir fluid were selected from reliable published data. The convergence behaviors of the new reduction technique for both samples are close to the full flash calculations according to the performed numerical experiments. The calculated equilibrium ratios and phases mole fractions for the reduced set of equations are very close to the results calculated for the conventional approach. The approach implementation procedure is simple and straightforward. This means that with full set of equilibrium equations and their corresponding derivatives, the reduced equation and their derivatives with respect to solution variables can be obtained, and there is no considerable difficulty regarding implementation. The method development was based on the compressibility and fugacity

coefficients of Peng-Robinson equation of state; however, the approach is general and can be applied to any two-parameter cubic equation of state.

NOMENCLATURE

AAD%   Average absolute deviation percent

A, B   EOS capital attraction repulsion parameters

a, b   EOS small attraction repulsion parameters

AD%   Absolute deviation percent

AF   Acentric factor

CAR   Cumulative absolute residual

EOS   Equation of state

f   Fugacity

G   Residual equation

K   Equilibrium ratio

J   Jacobian Matrix

MW   Molecular weight

P   Pressure

P_c Critical pressure

T   Temperature

T_c Critical temperature

V_c Critical Volume

Z   Compressibility factor

nv   Phase mole fraction

ζ   Solution variable

ω   Acentric factor

x_i^p Component mole fraction for phase p

x_i, y_i Phases mole fraction

μ_i Chemical potential

ϕ_i Fugacity coefficient

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APPENDIX

To calculate the required EOS derivatives for the full and reduced flash, the compressibility factor derivatives can be written as:

$$\frac{\partial Z^p}{\partial x^P_i} = \frac{\partial Z^p}{\partial A^p}\frac{\partial A^p}{\partial x^P_i} + \frac{\partial Z^p}{\partial B^p}\frac{\partial B^p}{\partial x^P_i} \tag{1}$$

The compressibility factor derivatives can be formulated as:

$$\frac{\partial Z^p}{\partial A^p} = -\frac{Z^p - B^p}{3Z^p.Z^p - 2Z^p(1-B^p) + A^p - 2B^p - 3B^p.B^p} \tag{2}$$

$$\frac{\partial Z^p}{\partial B^p} = -\frac{Z^p.Z^p - 2Z^p - 6Z^pB^p - A^p + 2B^p + 3B^p.B^p}{3Z^p.Z^p - 2Z^p(1-B^p) + A^p - 2B^p - 3B^p.B^p} \tag{3}$$

The derivative of compressibility factor for each phase with respect to capital EOS parameters for PR must be calculated implicitly:

$$\frac{\partial B^p}{\partial x^P_i} = \frac{\partial b^p / \partial x^P_i}{RT} \tag{4}$$

$$\frac{\partial A^p}{\partial x^P_i} = \frac{\partial a^p / \partial x^P_i}{(RT)^2} \tag{5}$$

The capital EOS parameters derivatives with respect to phase composition are defined by:

$$\frac{\partial a^p}{\partial x^P_i} = 2.a_i^{0.5}\sum_j x_j a_j^{0.5} \tag{6}$$

$$\frac{\partial b^p}{\partial x^P_i} = b_i \tag{7}$$

Using the above derivatives, the fugacity coefficient derivatives with respect to composition can be calculated as:

$$\frac{\partial Ln\varphi_i^p}{\partial x_j^L} = \frac{\partial A^P_1}{\partial x_j^p} + \frac{\partial A^P_2}{\partial x_j^p}b_i + \frac{\partial A^P_i}{\partial x_j^p}a^{0.5} \tag{8}$$

In this relation each term is defined as following:

$$\frac{\partial A^p_1}{\partial x_i^p} = -\frac{\left(\partial Z^p / \partial x_i^p - \partial B^p / \partial x_i^p\right)}{\left(Z^p - B^p\right)} \tag{9}$$

$$\frac{\partial A^p_2}{\partial x_j^p} = \frac{\left(b^p\partial Z^p / \partial x_j^p - Z^p\partial b^p / \partial x_j^p\right)}{b^p.b^p} +$$
$$+\frac{B^p b^p\partial A^p / \partial x_j^p - A^p\left(b^p\partial B^p / \partial x_j^p + B^p\partial b^p / \partial x_j^p\right)}{B^p.B^p.b^p.b^p p_1}Ln\left(\frac{Z^p + B^p p_2}{Z^p + B^p p_3}\right)$$
$$+\frac{A^p}{B^p p_1}\left(\frac{\partial Z^p / \partial x_j^p + p_2\partial B^p / \partial x_j^p}{Z^p + B^p p_2} - \frac{\partial Z^p / \partial x_j^p + p_3\partial B^p / \partial x_j^p}{Z^p + B^p p_3}\right) \tag{10}$$

where,

$$LnZEDB^p = Ln\left(\frac{Z^p + B^p p_2}{Z^p + B^p p_3}\right) \tag{11}$$

$$\begin{bmatrix}\frac{\partial A^p_3}{\partial x_j^p} = -\left(\frac{B^p\partial A^p / \partial x_j^p - A^p\partial B^p / \partial x_j^p}{B^p p_1}\left(\frac{2s^p}{a^p}\right)LnZEDB^p\right)\\ -\frac{A^p}{B^p p_1}\left(\frac{2a^p\partial s^p / \partial x_j^p - 2s^p\partial a^p / \partial x_j^p}{a^p.a^p}\right)LnZEDB^p\\ -\frac{A^p}{B^p p_1}\left(\frac{2s^p}{a^p}\right)\left(\frac{\partial Z^p / \partial x_j^p + p_2\partial B^p / \partial x_j^p}{Z^p + B^p p_2} - \frac{\partial Z^p / \partial x_i^p + p_3\partial B^p / \partial x_j^p}{Z^p + B^p p_3}\right)\end{bmatrix} \tag{12}$$