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ORIGINAL PAPER - PRODUCTION ENGINEERING

An improved component retrieval method for cubic equations of state with non-zero binary interaction coefficients for natural oil and gas

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Abstract Volumetric and equilibrium calculations for the natural gas and oil defined by a large number of components are not feasible in applications like compositional reservoir simulation. Therefore, the fluid mixture is grouped to reduce computational load and to make faster calculations. However, for several reasons, it is required to have the detailed fluid composition rather than the lumped one. In this work, an improved delumping method is presented to retrieve the phase composition of the detailed mixture based on the grouped mixture thermodynamic calculations. The method is based on previously proposed delumping techniques for non-cubic equation of state (Assareh et al. in Fluid Phase Equilib 339:40–51, 2013). To prepare lumped mixtures, a grouping technique, based on the components similarity, is used to classify the components with close critical properties and binary interaction coefficients in a pseudo-component (Assareh et al. in Int J Oil Gas Coal Technol 7(3):275–297, 2014). Afterward, a number of delumping parameters calculated from lumped system flash calculation are assigned to the components in a specific pseudo-component. The detailed mixture equilibrium ratios based on fugacity coefficient for a common cubic equation of state are calculated using these delumping coefficients. The accuracy of the method is verified on two petroleum reservoir fluids, a gas condensate and an oil reservoir fluid. The delumped equilibrium ratios were in good agreement with detailed ones with the absolute deviation of less than 2 %. The results confirm the applicability and accuracy of the presented method for detailed composition retrieval while simulating with pseudo-components.

Keywords Petroleum fluid characterization · Component retrieval · Equation of state · Lumping · Phase behavior · Cubic EOS

Abbreviations

AAD %	Average absolute deviation percent
E	Extended analysis
L	Lumped analysis
MW	Molecular weight
y_i	Mole fraction
f_i	Fugacity
ϕ_i	Fugacity coefficient
K_i	Equilibrium ration
T	Temperature (K, C)
P	Pressure (KPa)
T_C	Critical temperature (K)
V_C	Critical volume [m^3/Kmol]
P_C	Critical pressure (MPa)
w	Acentric factor
EOS	Equation of state
Ω_{del}	Value in the lumped system
Ω_{det}	Value in the extended system

Introduction

Petroleum reservoirs' fluids composition undergoes considerable changes through the field exploitation (Danesh et al. 1992; Kuntadi et al. 2012; Rastegar and Jessen 2009).

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This composition modification, resulted from different oil and gas velocities in porous medium for regular production scenarios. Reservoir fluid type and its thermodynamic condition may enhance the composition change. For example, volatile oil and gas condensate reservoir fluids experience larger composition changes for the same production scenarios than dry gas and black oil reservoir fluids. This phenomenon is accelerated in the case of gas injection processes wherein hydrocarbons and non-hydrocarbons with different compositions are mixed with in-place reservoir fluids. There are many components in petroleum reservoir fluids. These components are usually grouped due to computational resource limitations and calculation performance. In a typical grouping technique, grouped reservoir fluids are prepared in two steps. In the first step, components should be classified into different groups and in the second step, the pseudo-components (groups) critical and thermo-physical properties are calculated (Briesen and Marquardt 2004). Reservoir fluid composition plays a key role in properties' calculations. Therefore, oil and gas fields compositional simulation with grouped reservoir fluid descriptions lose their validity after a period (as pseudo-components properties are changing with composition change). Therefore, it is necessary to prepare a grouped fluid description for which composition changes have minimal impact to pseudo-components' properties. Besides this, detailed composition changes must be controlled to check the accuracy of the compositional simulation with a lumped fluid description. In addition, there are several cases in which it is required to retrieve the detailed fluid composition from equilibrium calculations performed on lumped fluid description (Kuntadi et al. 2012). For example, to simulate a surface facility, for which the inputs are the compositions of the reservoir outputs provided by the reservoir simulation, those must usually be known with precision. Surface facility simulations can be performed for a larger number of components (Nichita et al. 2007; Nichita and Graciaa 2011). The detailed equilibrium ratios' estimation from the results of a lumped system flash calculation is referred to as delumping or inverse lumping process (Schlijper and Drohm 1988). Several delumping methods are reported in the literature for cubic equations of state like Peng–Robinson (PR) (Peng and Robinson 1976).

Danesh et al. (1992) implemented a modified Wilson equation for K value variations as a function of equations of state (EOS) parameters (Danesh et al. 1992). In their work, they mentioned that in gas-injection processes in which fluid compositions vary considerably, the use of group properties commonly generated from the original oil composition is inaccurate for prediction of the phase behavior. They made composition retrieval of each phase after equilibrium calculations and formed the new groups for the next cell calculations in a reservoir simulator. In this delumping approach, they determined the constants by nonlinear least squares for the lumped equilibrium data. The original component K values were subsequently determined from the equation to retrieve the detailed compositions of the relevant phases. They have presented the application of this method for gas injection processes simulation. Based on this, they tracked the overall composition using material balance calculations. They expressed the log of equilibrium ratio as a linear function of:

$$\mathrm{Ln}K_i = c_0 + c_1(1+\omega_i)\left(1-\frac{1}{\mathrm{Tr}_i}\right), \tag{1}$$

where ω_i is the component acentric factor and Tr_i is the reduced temperature, while c_0 and c_1 are constants determined from equilibrium information from lumped fluid equilibrium calculations.

Stenby et al. (1996) proposed a delumping method for a two-ase flash calculation. The idea was to analyze the fugacity coefficients derived from EOS according to Michelsen reduction approach (Michelsen 1986; Stenby et al. 1996). In this method, a flash calculation is performed on the lumped system to obtain the lumped component equilibrium ratios. The delumping coefficients calculated from a regression technique are determined within flash calculation on lumped system, using the equilibrium ratios of the pseudo-components and the EOS parameters. Finally, the detailed equilibrium ratios were calculated according to these coefficients. They defined equilibrium ratios as:

$$\mathrm{Ln}K_i = \Delta c_0 + \Delta c_1\sqrt{a_i} + \Delta c_2 b_i. \tag{2}$$

In this equation, Δc_0, Δc_1 and Δc_2 are constants and a_i and b_i are attraction and repulsion parameters, respectively. When all binary interaction parameters are zero, these parameters are calculated analytically, otherwise this equation is an approximation and the three mentioned constants are calculated from curve fitting (Leibovici et al. 1996). Since then, several authors implemented this delumping algorithm for detailed component retrieval in compositional simulation. They used this algorithm in each time step to calculate the detailed phase's composition in each grid block and in well stream (Barker and Leibovici 1999; Vignati et al. 2009; Leibovici et al. 2000).

In this work, an improved delumping technique is introduced with the purpose to achieve more precision for detailed components' retrieval. The technique is based on the method proposed by Stenby et al. (1996) for inverse lumping (Stenby et al. 1996). Assareh et al. (2013) proposed a technique for delumping with non-cubic equations of state with non-zero interaction coefficients (Assareh et al. (2013). With this background, the proposed method for this work includes detailed mixture components'

classification into pseudo-components by a clustering technique and pseudo-components' properties calculation using mixing rules. The clustering technique is performed in a way that the components with similar properties (also with close binary interaction coefficients) are grouped together. The mentioned clustering technique is extensively examined in the work of Assareh et al. (2014). Afterward, a two-phase flash calculation is performed on the lumped mixture. At the end of flash calculation, a set of delumping coefficients is calculated for each phase for detailed system components' retrieval. The number of the delumping coefficients in this approach depends on the number of single/pseudo-components present in the mixture lumped fluid description. Compared with Lebovinci–Stenby–Knudsen (LSK), there is no regression required for equilibrium ratios calculation constants. Instead the delumping coefficients are increased from three to the number of single/pseudo-components in the lumped fluid description. The exactness of the method is then examined over two real reservoir fluid samples published in the literatures. The method is also compared with two frequently used techniques in this area. Finally, a brief discussion of the results is given. Even though the method is developed for PR equation of state, the general workflow is applicable to the common cubic equations of state in chemical and petroleum industries.

Peng–Robinson equation of state

The cubic EOS are frequently used in petroleum and chemical industries. These equations can be written as:

$$Z^3 + sZ^2 + qZ + r = 0, \tag{3}$$

where:

$$s = (u-1)B - 1, \tag{4}$$

$$q = A + (w-u)B^2 - uB, \tag{5}$$

$$r = -AB - wB^2 - wB^3. \tag{6}$$

Different cubic equations of state have different u and w values, and they also use different relations to calculate parameters a_i and b_i of each component. For the PR equation u is 2 and w is -1. The attraction and repulsion terms are:

$$a_i = \frac{0.4572R^2T_{c_i}^2\left[1+f_w\left(1-\left(\frac{T}{T_{c_i}}\right)0.5\right)\right]^2}{P_{c_i}}, \tag{7}$$

where

$$f_w = 0.37464 + 1.54226w_i - 0.26992w_i^2, \tag{8}$$

and

$$b_i = \frac{0.0778RT_{c_i}}{P_{c_i}}, \tag{9}$$

where T_{C_i} and P_{C_i} are the critical temperature and critical pressure of each component, T is the reservoir temperature, and w_i is the acentric factor of each component (Walas 1985). The mixture parameters are then defined as:

$$a = \sum_i \sum_j x_i x_j \sqrt{a_i a_j}\,(1-k_{ij}), \tag{10}$$

$$b = \sum_i x_i b_i. \tag{11}$$

From which A and B are defined as:

$$A = \frac{aP}{R^2T^2}, \tag{12}$$

$$B = \frac{bP}{RT}. \tag{13}$$

For delumping evaluations, the binary interaction coefficients, both for extended analysis and the clustered analysis of the mixture, are calculated from:

$$k_{ij} = 1 - \left(\frac{2v_{c_i}^{1/6}v_{c_j}^{1/6}}{v_{c_i}^{1/3}+v_{c_j}^{1/3}}\right)^{\theta}, \tag{14}$$

where v_{c_i} is the critical volume of component i, and θ is the hydrocarbon–hydrocarbon interaction coefficient exponent. It has been shown that a value of 1.2 provides a good match of the paraffin–paraffin interaction.

Delumping technique

The basic idea of the delumping calculation is to separate the PR EOS inputs (a_i, b_i) for each lumped component from delumping coefficients in the fugacity coefficient formulations, where the binary interaction coefficients are zero. The zero interaction coefficients ensure that the fugacity coefficient terms are not explicit function of composition as a result of mixing rules. It means that, in case one reaches to system with close thermodynamic behavior to this system (which is a lumped mixture), theses delumping coefficients are similar in both systems. It is then sufficient to calculate the fugacity coefficients from the delumping coefficients calculated from lumped system in a two-phase flash calculation multiplied by PR input parameters for the detailed mixture components. In this approach at first, a lumped system with lower number of the components is desired. The thermodynamic behavior of the lumped system must be close to one of the detailed systems as much as possible. Then, a two-phase flash calculation is performed on the lumped system. After

the convergence of the lumped system flash problem, the delumping coefficient arrays for liquid and gas phases are calculated.

Within this framework, the detailed system equilibrium ratios and components' retrieval are achieved. If there is no difference between lumped and detailed mixture regarding thermodynamic and volumetric behavior, the delumped equilibrium ratios are the same as equilibrium ratios calculated from a two-phase flash calculation with detailed system. The higher the difference between lumped and detailed system, the higher is the difference between delumped and detailed K values. The phase properties, in which there is no mole fraction expressed explicitly, are equal for lumped and delumped system. This approach can be also generalized to include delumping for a system with non-zero binary interaction coefficients. In this respect, the mole fraction dependent pseudo-components delumping coefficients are valid for comprising components. These include compressibility factor, A, B, a, b and so on. Having the fugacity coefficient of the components in each phase from the PREOS:

$$\mathrm{Ln}\varphi_i^P = \frac{b_i}{b}(Z-1) - \mathrm{Ln}(Z_P - B_P) - \frac{A_P}{B_P\sqrt{u^2-4w}}\left(\frac{b_i}{b_P} - \frac{1}{a_P}\frac{\partial a_P}{\partial x_i}\right)\mathrm{Ln}\left(\frac{2Z_P + B_P\left(u+\sqrt{u^2-4w}\right)}{2Z_P + B_P\left(u-\sqrt{u^2-4w}\right)}\right) \quad (15)$$

The delumping coefficients array for each phase is defined as:

$$DA = [DA_1, DA_2, \ldots, DA_i, \ldots, DA_{n_l}], \quad (16)$$

where n_l is the number of lumped system components. The entries of this vector are then calculated:

$$DA_1 = -\mathrm{Ln}(Z_\mathrm{P} - B_\mathrm{P}), \quad (17)$$

$$DA_2 = \left(\frac{Z_\mathrm{P}-1}{b_\mathrm{P}}\right) - \frac{A_\mathrm{P}}{B_\mathrm{P}\sqrt{u^2-4w}}\frac{1}{b_\mathrm{P}}\mathrm{Ln}\left(\frac{2Z_\mathrm{P} + B_\mathrm{P}\left(u+\sqrt{u^2-4w}\right)}{2Z_\mathrm{P} + B_\mathrm{P}\left(u-\sqrt{u^2-4w}\right)}\right), \quad (18)$$

$$DA_{i+2} = \left(\frac{1}{a_\mathrm{P}}\frac{A_\mathrm{P}}{B_\mathrm{P}\sqrt{u^2-4w}}\right)\mathrm{Ln}\left(\frac{2Z_\mathrm{P} + B_\mathrm{P}\left(u+\sqrt{u^2-4w}\right)}{2Z_\mathrm{P} + B_\mathrm{P}\left(u-\sqrt{u^2-4w}\right)}\right) \times \left(\frac{\partial a_P}{\partial x_i}/\sqrt{a_i}\right), \quad i = 1 : n_\mathrm{c} \quad (19)$$

where the derivative of the attraction term with respect to phase composition is:

$$\frac{\partial a_P}{\partial x_i} = 2\sqrt{a_i}S_i^P, \quad (20)$$

$$S_i^P = \sum_{j=1}^{n_\mathrm{c}} x_j(1-k_{ij})\sqrt{a_j}. \quad (21)$$

If there are no non-zero binary interaction coefficients in the lumped fluid description, the delumping array elements from the third element until the end are the same. If the components classified as a pseudo-component have close binary interaction coefficients, S_i^P for each pseudo-component is valid for the component comprising it. Therefore, it is important that the components grouped as a pseudo-component have similar interaction coefficients with important mixture components (those components with higher interaction coefficient and higher impact on the phase behavior). In the case of non-zero binary interaction coefficients, each array element from the third array entry is used for the corresponding pseudo-component and is used to calculate the detailed equilibrium ratios for the components comprising that pseudo-component. Therefore, we have delumping coefficient equal to lumped fluid description components number plus two. A flow diagram of the proposed delumping technique is shown in Fig. 1. The first two delumping array elements are the same for all single components and pseudo-components available in the lumped fluid description. From the third element until the end of an array, each element corresponds to components (single and pseudo-components). These elements are the same for those single/pseudo-components with zero binary interaction coefficients with other components in lumped fluid

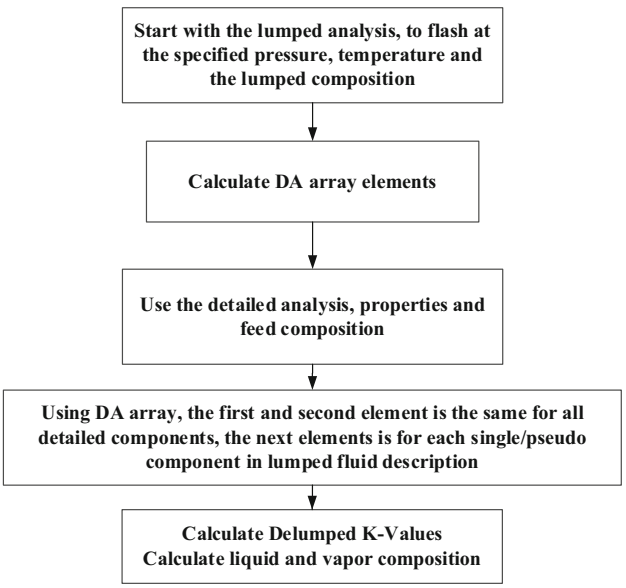

Fig. 1 Flow diagram of the delumping method 19

description. In this step, each single/pseudo-component in the lumped fluid description has three delumping coefficients: the first two are the same and the third is only the same for those components with zero binary interaction coefficients to other components. In the second step, equilibrium ratios for the detailed components are calculated using attractions and repulsion parameters (a_i and b_i) and three delumping coefficients for components comprising the related single/pseudo-component. This means that compared with LSK, there is no regression required for equilibrium ratios calculation constants. Instead, the delumping coefficients are increased from three to the number of single/pseudo-components in the lumped fluid description. Not all the lumping schemes available in the literatures can be used to prepare the lumped mixture for this delumping technique, if accuracy of the component retrieval is important. There is a clear constraint to select the lumping method. It should classify the components with close critical properties (which can ensure close binary interaction coefficients as a byproduct). In this work, the pseudo-component generation proposed by Assareh et al. (2014) is used to prepare the grouped system (Assareh et al. 2014). In this technique, the mixture components are classified with a fuzzy clustering algorithm. For the pseudo-components' properties, an EOS-based mixing rule is applied which is described in (Assareh et al. 2014) A grouped mixture must reproduce the same EOS parameters as detailed mixture ideally. This concept is served as the basis for the calculation of critical pressure and critical temperature.

Results and discussion

The proposed delumping technique was applied to component retrieval for two real petroleum fluid samples. Sample 1 is an oil reservoir mixture from Stenby et al. (1996). The extended analysis is described by ten individual components and ten fractions, in which the heaviest being C_{48+}. The data for sample 2 are obtained from North Sea gas condensate by Leibovici et al. (1993) including 27 components (Leibovici et al. 1996). The first step in the evaluation of delumping scheme is to examine the prepared lumped fluid description. The fluid phase behavior must be analyzed to investigate the proposed groups under physical feedback for different numbers of groups. The phase envelope (PT diagram), differential liberation (DL) for oil mixture and constant volume depletion (CVD) for gas condensate were used for this purpose. For the comparison between simulated experimental result, the below definition is valid:

$$\mathrm{AAD}\,\% = \frac{1}{n_{\mathrm{step}}}\sum_{i}^{n_{\mathrm{step}}}\left|\frac{\Omega^{\mathrm{det}}-\Omega^{\mathrm{del}}}{\Omega^{\mathrm{det}}}\right|_i \times 100 \tag{22}$$

In relation, n_{step} is the number of the pressure steps in the PVT experiment. For comparison of the detailed and delumped equilibrium ratios, the AD % is defined as follows:

$$\mathrm{AD}\,\% = \left|\frac{\Omega^{\mathrm{det}}-\Omega^{\mathrm{del}}}{\Omega^{\mathrm{det}}}\right| \times 100 \tag{23}$$

Therefore, the average of absolute deviation percent on the components is

$$\mathrm{AAD}\,\% = \frac{1}{n_{\mathrm{c}}}\sum_{i}\left|\frac{\Omega^{\mathrm{det}}-\Omega^{\mathrm{del}}}{\Omega^{\mathrm{det}}}\right|_i \times 100 \tag{24}$$

The suggested technique was also compared for two frequently used techniques to prove its exactness and efficiency. For oil reservoir fluid, the components in the detailed reservoir fluid description, from IC4 to C38, were lumped to prepare six pseudo-components using Assareh et al. (2014) clustering approach. This means that the system components' number is reduced from 20 to 11. Those components were placed in a pseudo-component, which had critical and thermo-physical properties close to each other. The generated groups are presented in Table 1. Figures 2 and 3 show the quality of the lumped fluid description. Figure 2 presents comparison between PT diagram for extended analysis and clustered mixture. In the DEW line, critical point and low pressure bubble line, the curves confirm a perfect agreement between original and characterized mixture. Figure 3 shows the result of a simulated DL test for gas oil ratio and gas compressibility

Table 1 Pseudo-components generated for the oil reservoir fluid mixture components

	Mole frac	V_{C} (m^3/Kmol)	T_{C} (K)	AF	MW	P_{C} (BAR)	Components
PS1	0.020	0.280	438.707	0.209	64.633	35.497	IC4, NC4, IC5, NC5
PS2	0.141	0.399	562.925	0.504	110.074	29.048	C6, C7
PS3	0.110	0.606	646.931	0.691	175.272	20.588	C11, C14
PS4	0.094	0.772	723.316	0.883	254.577	16.791	C16, C20
PS5	0.062	0.888	810.122	1.107	364.213	14.890	C23, C27
PS6	0.041	0.979	919.421	1.307	524.236	14.008	C32, C38

The table shows critical properties and composition of each pseudo-component and its comprising components

factor. The average deviation percent for gas oil ratio over the pressure steps in the DL test is 0.4 % and for gas compressibility factor, 0.08 %. To examine the delumping technique, the composition of the fluid at pressure stage of 24,000 (KPa) was taken to retrieve the oil and gas detailed phase composition. The delumped equilibrium ratios were plotted versus the detailed one in Fig. 4 with an R^2 error of 1. Figure 5 shows the oil and gas phase composition compared with the phase composition calculated with flash calculation on the detailed system.

For the gas condensate reservoir fluid, the components from IC4 to AC9 were grouped into four pseudo-components.

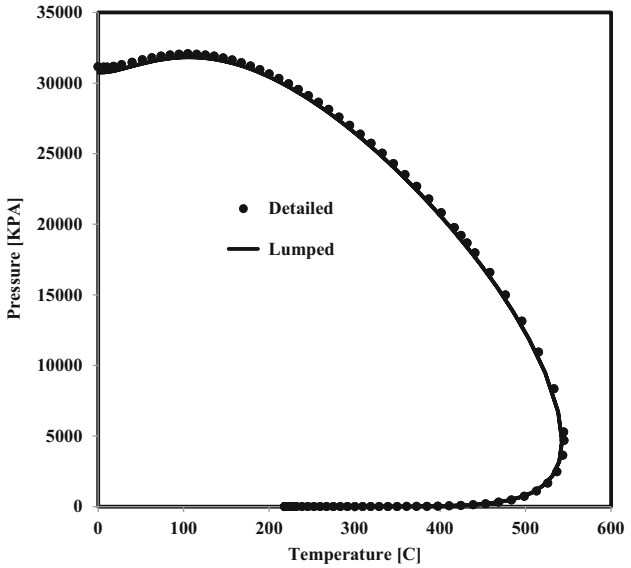

Fig. 2 Phase envelope for detailed (Det) and lumped (Lump) mixture, oil reservoir fluid 20

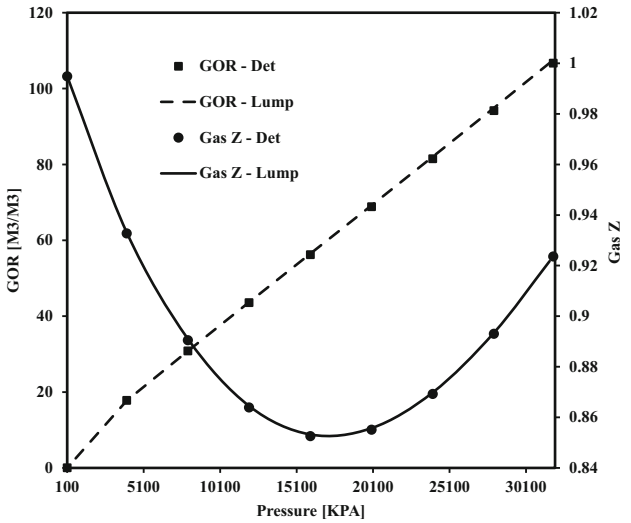

Fig. 3 Gas oil ratio (GOR) and gas compressibility factor (GAS Z), for the lumped and delumped system in a DL test performed at 71.11 (C), oil reservoir fluid 21

The components in the original mixture were clustered from 27 to 11 groups. The generated lumped components and their properties are described in Table 2. The quality of the lumped mixture was examined over phase-behavior calculations. Figure 6 shows the phase envelope comparison between detailed and lumped fluid descriptions. The results of simulated CVD, test for the liquid dropout and gas compressibility factor are shown in Fig. 7. It is deduced from Fig. 7 that the phase behavior of the system with generated pseudo-components is

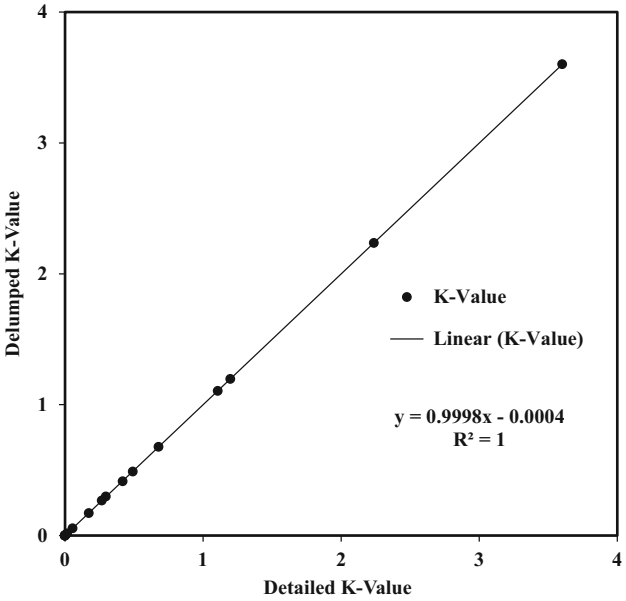

Fig. 4 *K* value at pressure stage of 24,000 (KPA) for the DL test performed at temperature of 71.11 (C), comparison of detailed and delumped analysis, oil reservoir fluid 22

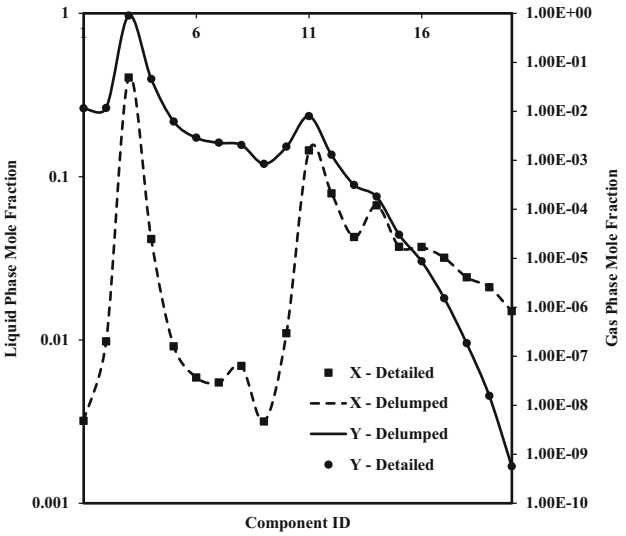

Fig. 5 Liquid phase mole fraction (X) and gas phase mole fraction (Y) at pressure stage of 24,000 (KPA) for the DL test performed at temperature of 71.11 (C), Comparison of detailed and delumped analysis, oil reservoir fluid 23

Table 2 Pseudo-components generated for the gas condensate mixture components

	Mole frac	V_C (m^3/Kmol)	T_C (K)	AF	MW	P_C (BAR)	Components
PS1	0.030	0.276	439.891	0.203	63.791	36.267	IC4, NC4, IC5, NC5, CC5
PS2	0.020	0.328	552.493	0.246	89.702	37.785	PC6, CC6, AC6, CC7, AC7
PS3	0.011	0.413	582.725	0.302	107.540	31.060	PC7, CC8, AC8, AC9
PS4	0.011	0.507	604.632	0.392	128.790	25.524	PC8, PC9, CC9, PC10, CC10, AC10

The table shows critical properties and composition of each pseudo-component and its comprising components

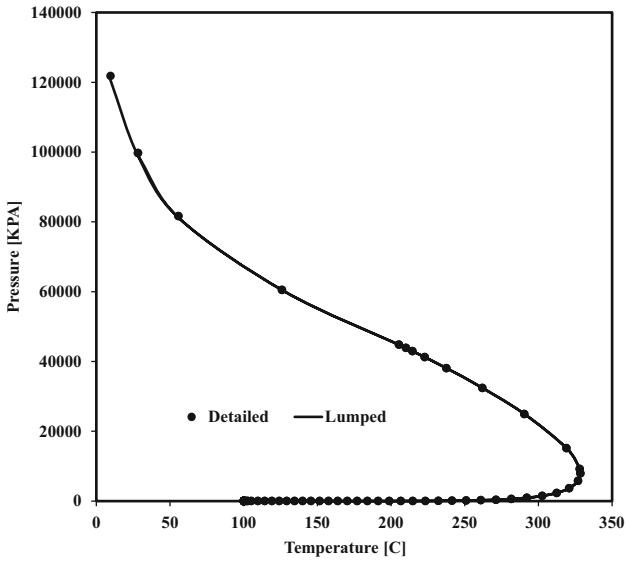

Fig. 6 Phase envelope for detailed and lumped mixture, gas condensate reservoir fluid 24

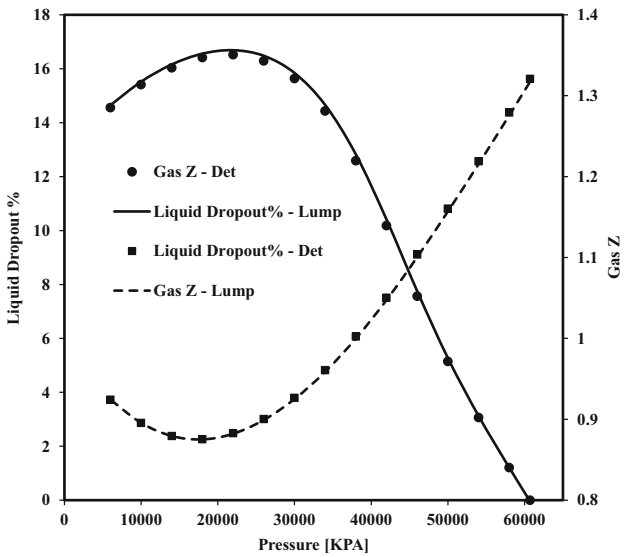

Fig. 7 Liquid dropout % and gas compressibility factor in the CVD test performed at temperature of 125 (C), comparison of detailed and lumped mixture, gas condensate reservoir fluid 25

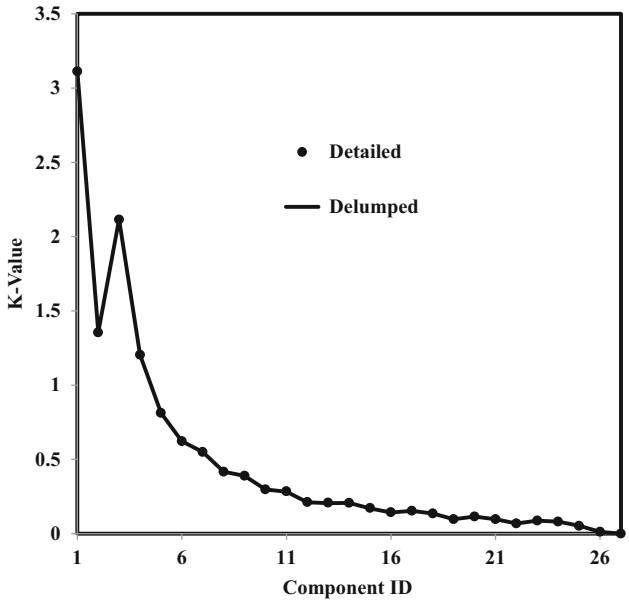

Fig. 8 Comparison of the detailed and delumped *K* value at one of the CVD test stages [pressure 22,000 (KPA)] performed at 71.11 (C), gas condensate reservoir fluid 26

close to the detailed system phase behavior. The average of absolute deviation for the gas compressibility factor is 0.158 % and for the liquid volume dropout is 1.38.

The delumping technique was performed on the mixture taken from CVD test at pressure stage of 22,000 (KPa). The equilibrium ratios for delumped and detailed calculation are plotted for each component in Fig. 8. The average of absolute deviation of the delumped k values and the detailed ones is less than 0.6 %.

The delumping technique was also compared with two common lumping techniques, Danesh et al. (1992) and LSK (Stenby et al. 1996), based on the same lumped system, in Table 3. The table shows good performance in comparison to the other delumping techniques. In this table, the average of absolute deviation between detailed and delumped equilibrium ratios for all components is 0.237 for the proposed technique, 11.046 for Danesh method and 2.243 for LSK approach. This shows acceptable accuracy of the proposed technique. This accuracy is related to the fact that the LSK approach uses three

Table 3 Comparison of the AAD % for the *K* value for different delumping methods, 405 (BAR), 130 (C)

Components	Detailed	A—AD %	B—AD %	C—AD %
N_2	1.757	0.235	19.392	0.012
CO_2	1.132	0.104	2.677	0.725
C_1	1.434	0.175	12.923	1.251
C_2	1.083	0.096	1.906	0.432
C_3	0.897	0.044	3.407	1.303
iC_4	0.792	0.058	6.460	2.011
nC_4	0.741	0.039	7.006	1.548
iC_5	0.652	0.018	9.386	2.094
nC_5	0.630	0.011	9.989	2.273
CC5	0.531	0.058	9.793	0.288
PC6	0.545	0.737	12.175	2.917
CC6	0.450	0.620	9.860	1.057
AC6	0.436	0.540	12.209	1.176
PC7	0.467	0.066	13.741	3.245
CC7	0.410	0.708	9.996	1.568
AC7	0.365	0.633	10.468	1.708
PC8	0.407	0.067	15.741	4.510
CC8	0.370	0.011	11.561	0.460
AC8	0.303	0.071	9.225	3.788
PC9	0.355	0.061	17.037	5.342
CC9	0.312	0.010	11.114	1.602
AC9	0.256	0.086	8.160	5.276
PC10	0.314	0.063	19.013	7.249
CC10	0.289	0.012	11.588	1.247
AC10	0.225	0.089	7.527	5.986
CN-1	0.117	0.573	9.428	0.350
CN-2	0.016	1.212	26.450	1.142
AAD %	0.0	0.237	11.046	2.243

The detailed equilibrium ratios are specified under detailed column. The other columns show the absolute average deviation of the delumping methods A, B and C, respectively, for the newly developed method, Danesh method and Leibovinci–Stenby–Knudsen method. The last row shows the average of the deviation overall components

regressed coefficients to calculate the detailed equilibrium ratios while in the proposed approach for this work, the number of delumping coefficients depends on the number of pseudo-components.

Conclusion

A new delumping technique was developed and tested on the real petroleum fluid mixtures. The fluid mixtures were initially lumped with a clustering technique. Afterward, a two-phase flash calculation was performed on the lumped systems to calculate some delumping coefficients in each phase. The delumping coefficients for each pseudo-component are then assigned to the components comprising it for each phase. In this regard:

- The quality of the proposed delumping technique is related to the quality of the lumping technique.
- The method helps to have less computational load while providing detailed phase information with acceptable estimation.
- The absolute average percent for proposed delumping method is less than 2 %.
- This work flow is applicable to the common equations of state in chemical and petroleum industries.

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