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Research Note

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Improved Phase Behavior Calculations of Reservoir Fluids Using a New Distribution Model

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In this paper, the distribution model for C_{7+} fractions proposed by Riazi [1] has been used with combined Peng-Robinson and modified Redlick-Kwong equations of state for prediction of phase and volumetric behavior of reservoir fluids. A computational method is presented for property and phase equilibrium calculation of petroleum fluids. The method is based on the use of a distribution function to define pseudocomponents for the hydrocarbon plus-fraction of the petroleum fluid. The calculation procedure is demonstrated by calculating the composition and specific gravity of the stock-tank oil as well as GOR and saturation pressure for a reservoir fluid from the Middle East fields.

INTRODUCTION

The Vapor-Liquid Equilibrium (VLE) calculations, such as isothermal flash, bubble/dew points pressure and Gas-to-Oil Ratio (GOR), are important in petroleum production, processing and transportation. For example, volumetric properties such as density, are important in the calculations related to fluid flow, fugacity or transport properties.

Naturally occurring petroleum fluids known as reservoir fluids, are complex mixtures of hundreds of compounds, including light and intermediate hydrocarbons, a few non-hydrocarbons (i.e. H_2S, N_2, CO_2 and H_2O) and a large number of heptanes and heavier compounds (C_{7+}). Laboratory analysis of such reservoir fluids usually give a limited description of the heavy components. Hydrocarbons heavier than hexane are normally lumped into a C_{7+} fraction with measured molecular weight (M_{7+}) and specific gravity (S_{7+}).

The major difficulty in prediction of phase behavior and properties of reservoir fluids and crude oils is in the characterization of its C_{7+} fraction. Calculations show that treating the whole C_{7+} fraction as one pseudo-component is not, perhaps, accurate, at least for heavier reservoir fluids [2]. To overcome this difficulty, at least two approaches are available in the literature. The first approach is to treat C_{7+} as a continuous mixture of Single Carbon Number (SCN) compounds through use of a probability density or a distribution function [3-8]. The second and more commonly used approach is to split the C_{7+} fraction into a number of subfractions or "pseudocomponents". This method of characterization of reservoir fluids has been in use for the past two decades [2,9-11].

Recently, Riazi [1] developed a new characterization scheme for C_{7+} fractions. The main purpose of this paper is to demonstrate the application of the previously developed distribution model in calculation of the phase behavior of reservoir fluids. Another difficulty arises in the use of cubic equations of state, due to their low performance in predicting liquid phase densities. Riazi et al. [12,13] modified the "b" parameter of the Redlich-Kowng Equation Of State (RK-EOS), in terms of molar refraction, which significantly improved liquid density predictions, specially for heavy hydrocarbons. Moreover, Riazi and Sahhaf [14] proposed certain correlations to improve estimation of the critical properties and acentric factors of heavy hydrocarbons and fractions. These are the specific features of the proposed calculation scheme for phase behavior and volumetric properties of reservoir fluids, which is presented in this paper.

PROPOSED CALCULATION SCHEME

In the application of a cubic equation of state to perform phase behavior calculations for reservoir fluids, one needs to accurately specify the composition and properties of components in the mixture, especially the heptane-plus fractions. In this paper, the distribution model for the C_{7+} characterization has the following

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probability density function [1]:

$$F(P^*) = \frac{B^2}{A} P^{*^{B-1}} \exp(-\frac{B}{A} P^{*^B}), \quad (1)$$

$$P^* = \frac{P - P_o}{P_o}, \quad (2)$$

where P is a property such as absolute boiling point (T_b), molecular weight (M) and specific gravity (S) or the refractive index parameter. In Equation 1, P^* is a dimensionless form of parameter P and P_o is a parameter specific for each property (T_o, M_o, S_o) and each mixture. P_o is, in fact, the value of P for the lightest component in the C_{7+} fraction. A and B in Equation 1 are two parameters specific to each property and each mixture. Riazi [1] outlines in detail how one can determine the distribution parameters A, B and P_o for M and S using the molecular weight and specific gravity of the C_{7+} fraction (M_{7+} and S_{7+}) as the minimum data available. It should be noted that parameter P^*, defined by Equation 2, varies from 0 to infinity for M, T_b and S. From the definition of P^* it is obvious that the probability density function, in terms of original parameter P, can be found by dividing $F(P^*)$ to P_o, that is $F(P) = F(P^*)/P_o$.

Once molar distribution in the form of Equation 1 is known, then two methods can be used to generate the pseudocompounds for the C_{7+} fraction. One method is to use the Gaussian quadrature method, as discussed by Stroud and Secrest [15]. The Gaussian quadrature method can be used to provide a discrete representation of continuous functions using different numbers of quadrature points. In the second method, for each pseudocomponent a range of molecular weights or carbon numbers is specified. For example, if the C_{7+} is divided into 5 pseudocomponents, carbon number ranges of C_7 - C_{10}, C_{11} - C_{15}, C_{16} - C_{25}, C_{26} - C_{35} and C_{36+} were found to be suitable ranges [1]. The molecular weight of each carbon number can be determined from the values provided by Riazi and Sahhaf [14]. From the probability density function given by Equation 1, one can determine the mole fraction, molecular weight, specific gravity and boiling point for each pseudocomponent.

In calculation of EOS parameters, one needs to estimate critical temperature, critical pressure, critical volume, acentric factor and the Binary Interaction Parameters (BIPs) for all the components in a defined mixture. Critical properties for pseudocomponents with molecular weights of less than 300 may be calculated from Riazi and Daubert [16,17], which are also included in the API-Technical Data Book [18]. For heavier compounds, relations developed by Riazi and Sahhaf [14], may be used. Hydrocarbon-hydrocarbon BIPs may be calculated from a modified relation proposed by Chueh-Prausnitz [19] while, for non-hydrocarbon-hydrocarbons, values suggested by Nagy and Shirkovskiy [20] can be used.

In the petroleum industry, both Soave (SRK) and Peng-Robinson (PR) equations of state are widely used [10,11]. In our calculations, the PR-EOS are used for estimation of fugacity and equilibrium ratios. Density and compressibility factors for each phase are calculated from the modified RK-EOS [12,13]. In this modified version of RK-EOS, parameter "b" from RK should be multiplied by a correction factor of β, which is given in the following relation.

$$\beta^{-1} = 1 + \{0.02[1 - 0.92\exp(-1000|T_r - 1|)] - 0.035(T_r - 1)\}(r - 1), \quad (3)$$

in which T_r is the reduced temperature. Parameter r is defined as the ratio of molar refraction (R_m) of the compound to that of methane, which is 6.987. Values of parameter r and its method of calculation are given by Riazi et al. [12,13]. One advantage of this equation is that parameter r can be determined accurately for heavy compounds [13]. Modified RK-EOS predicts liquid and vapor densities for hydrocarbons from C_1 to C_{40} and pressures up to 700 bar, with an average error of 1.4% for over 1700 data points. In addition, it significantly improves calculation of critical compressibility factors [13].

One unique aspect of this calculation scheme is that while the PR-EOS is used to estimate the fugacity coefficients, the compressibility factors calculated from the modified RK-EOS are used in the estimation of fugacity coefficients. If the only information available is the composition of light hydrocarbons up to C_6 and M_{7+} and S_{7+} of the C_{7+} fraction, then our calculation scheme can be summarized as follows:

- Generate 5 pseudocomponents for the C_{7+} fraction from Riazi's method [1];
- Obtain the critical properties from Riazi and Daubert [16,17] and for pseudocomponents with molecular weights greater than 300 from Riazi and Sahhaf [14];
- Calculate BIPs from the methods of Chueh-Prausnitz [19,20];
- Calculate fugacity coefficients from PR-EOS;
- Calculate densities and Z-factors from modified RK-EOS [12,13];
- Perform routine VLE calculations.

EVALUATION OF THE PROPOSED CALCULATION METHOD

Based on the calculation scheme presented above, a Fortran computer package was developed, which performs isothermal flash, saturation pressure, GOR and

Table 1. Experimental data for a Kuwaiti reservoir fluid in a three-stage separator test.

No.	Component	Feed	1st Stage Gas	2nd Stage Gas	3rd Stage Gas	3rd Stage Liquid
1	N_2	0.09	0.77	0.16	0.15	0.00
2	CO_2	2.09	4.02	3.92	1.41	0.00
3	H_2S	1.89	1.35	4.42	5.29	0.00
4	H_2O	0.00	0.00	0.00	0.00	0.00
5	C_1	29.18	63.27	31.78	5.10	0.00
6	C_2	13.60	20.15	33.17	26.33	0.19
7	C_3	9.20	7.56	18.84	36.02	1.88
8	nC_4	4.30	1.5	4.14	13.6	3.92
9	iC_4	0.95	0.43	1.24	3.62	0.62
10	nC_5	2.60	0.36	0.92	3.50	4.46
11	iC_6	1.38	0.24	0.63	2.46	2.11
12	C_6	4.32	0.24	0.57	2.09	8.59
13	C_{7+}	30.40	0.11	0.21	0.43	78.23
Sp. Gr. @ 60 F						0.8150
Temp.,°F		245	105	100	90	90
Pressure, psia		2387	315	75	15	15
GOR [scf/stb]		850	601	142	107	

density calculations for reservoir fluid. To demonstrate the proposed calculation scheme, a set of experimental data was used on Kuwaiti reservoir fluid in a three-stage separator test [21]. The feed composition, saturation pressure of the feed (bubble point), temperature and pressure, composition of gas and the GOR in each stage, as well as the liquid composition from the last stage, are all given in Table 1. Values of GOR are in standard cubic feet (at 1 atm. and 60°F) to one barrel of stock tank oil at 1 atm. and 90° F [SCF/STB].

The pseudocomponents generated for the C_{7+} fraction, with respective characterization and distribution parameters, are given in Table 2. Molar and specific gravity distributions of the C_{7+} fraction, in terms of density functions, are presented in Figure 1. Results of calculations for the proposed method and HYSYS are given in Tables 3 and 4, respectively. Predicted values for compositions of gases at each stage and the liquid product of the final stage, as well as GOR and liquid density, are in good agreement with the experimental data. Preliminary results show that the performance of this approach is better than the results obtained through existing commercial approaches [22]. For example, using such software, one can predict the

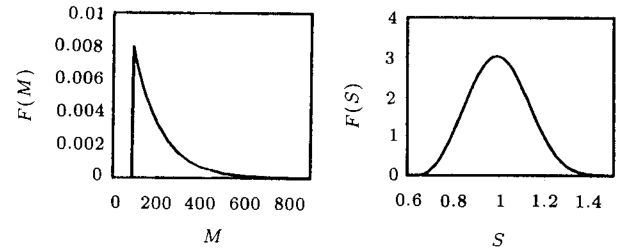

Figure 1. Probability density functions for molecular weight and specific gravity of the C_{7+} fraction in Table 2.

Table 2. Results for the C_{7+} characterization.

Pseudocomponent	Mol.%	Wt.%	Mol. Wt.	Sp. Gr.	T_b/K	n_{20}
C_{7+} (1)	10.0	12.5	110	0.750	391.8	1.419
C_{7+} (2)	9.0	17.1	168	0.810	487.9	1.450
C_{7+} (3)	7.7	23.1	263	0.862	602.1	1.478
C_{7+} (4)	2.5	11.6	402	0.903	709.0	1.501
C_{7+} (5)	1.2	8.2	608	0.949	777.6	1.538
Total C_{7+}	30.4	72.5	209.8	0.843	576.7	1.469

Experimental values on M_{7+} and S_{7+}:

$M_{7+} = 209.8$, $S_{7+} = 0.844$ and $n_{7+} = 1.4698$.

Distribution parameters and calculated values:

$M_o = 86.8$, $S_o = 0.65$, $B_M = 1$, $A_s = 0.119$, $A_M = 1.417$, $B_S = 3$, $M_{av} = 209.8$ and $S_{av} = 0.847$.

Table 3. Calculated values from the proposed technique for the data given in Table 1.

No.	Component	Feed	1st Stage Gas	2nd Stage Gas	3rd Stage Gas	3rd Stage Liquid
1	N_2	0.09	0.52	0.12	0.05	0.00
2	CO_2	2.09	3.90	4.09	1.44	0.02
3	H_2S	1.89	1.47	4.38	5.06	0.14
4	H_2O	0.00	0.00	0.00	0.00	0.00
5	C_1	29.18	63.88	32.12	5.68	0.03
6	C_2	13.60	19.90	32.65	25.41	0.38
7	C_3	9.20	7.40	18.24	35.47	3.05
8	nC_4	4.30	1.50	4.56	13.92	4.38
9	iC_4	0.95	0.43	1.23	3.47	0.78
10	nC_5	2.60	0.36	1.01	3.98	4.81
11	iC_6	1.38	0.24	0.68	2.61	2.37
12	C_6	4.32	0.27	0.61	2.22	9.01
13	C_{7+}	30.40	0.13	0.31	0.69	75.03
Sp. Gr. @ 60 F						0.8105
Temp.,°F		245	105	100	90	90
Pressure, psia		2197	315	75	15	15
GOR [scf/stb]		855	590	148	117	

Table 4. Calculated values from HYSYS simulator for the data given in Table 1.

No.	Component	Feed	1st Stage Gas	2nd Stage Gas	3rd Stage Gas	3rd Stage Liquid
1	N_2	0.09	0.20	0.03	0.002	0.00
2	CO_2	2.09	3.73	3.93	1.64	0.02
3	H_2S	1.89	2.44	4.77	4.95	0.19
4	H_2O	0.00	0.00	0.00	0.00	0.00
5	C_1	29.18	60.48	28.90	4.48	0.02
6	C_2	13.60	21.05	31.47	21.85	0.52
7	C_3	9.20	8.62	20.99	36.00	3.08
8	nC_4	4.30	1.84	5.32	15.87	4.88
9	iC_4	0.95	0.52	1.45	3.88	0.84
10	nC_5	2.60	0.44	1.27	4.62	4.85
11	iC_5	1.38	0.29	0.85	3.05	2.38
12	C_6	4.32	0.28	0.77	2.76	9.61
13	C_{7+}	30.40	0.11	0.25	0.89	73.61
Sp. Gr. @ 60 F						0.82
Temp.,°F		245	105	100	90	90
Pressure, psia		2197	315	75	15	15

mol% of C_{7+} in the 3rd stage liquid phase as 73.6 mol%, the specific gravity of the whole final liquid as 0.82 and the overall GOR as 840 scf/stb, while the actual values are 78.23, 0.8150 and 850, respectively (Table 1). The predicted mol% of C_{7+} in the 3rd stage liquid phase from the proposed method is 75.03%, the density from the proposed method for the final liquid product is 0.810, in terms of specific gravity at 60 F, while the calculated GOR is 855 scf/stb. In this case, improvement is not significant, mainly because the reservoir fluid is not heavy and no adjustment was used in the parameters. It is expected that the performance of the proposed method would be even better than existing methods for heavier reservoir fluids and could be further improved by adjusting one parameter, such as the binary interaction parameter. However, applicability of the method has been demonstrated in this paper. The effects of input data for BIPs, especially for heavy reservoir fluids, will be studied in future work.

CONCLUSION

A calculation scheme for estimation of phase split compositions, GOR, saturation pressure and liquid densities of reservoir fluids has been presented in this work. No adjustable parameter has been used in the proposed method. Results of calculations compare favorably with the experimental values demonstrating a sample performance for the proposed method. The proposed characterization scheme presented here can be implemented in commercial software to improve the prediction of nearly all thermodynamic and physical properties of reservoir fluids.

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