In compositional modeling, the phase characteristics and behavior of reservoir fluids are calculated using the equation of state. To simplify the calculations and speed them up, the components of the heptane plus fraction (C_{7+}) are grouped into pseudo-components. However, after this procedure, the results of compositional modelling of the reservoir containing the pseudo-components need to be delumped so that they can be used in surface models. It follows from this that the problem lies in the fact that the grouped composition cannot be applied to the modeling of ground structures. The object of the study is Kazakhstani oil, on the example of which a detailed component composition was obtained by analytical delumping based on reduction parameters. In laboratory conditions, the component composition of oil, and other fluid properties were determined. The study presents the results that prove the importance of applying the delumping algorithm in the context of compositional modeling. The results obtained analytically correspond quite accurately to the numerical calculations of the PVTsim software and laboratory experiments. A comparison of existing methods showed a difference of 5 %, which suggests that delumping is an excellent method for describing and obtaining a detailed composition of the hydrocarbon mixture. In practice, the results of the detailed composition of hydrocarbons can be used for the design of refineries. Also, the findings from this research can enhance the planning and design of surface facilities, particularly when developed under reservoir conditions where the pressure exceeds the saturation pressure

Keywords: delumping, lumping, pseudo-component, plus fraction, binary interaction parameters, K-value, equation of state, flash, compositional modeling, Kazakhstani oil

IMPROVEMENT OF THE DELUMPING METHOD IN ORDER TO OBTAIN DETAILED CHARACTERISTICS OF THE FLUID

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1. Introduction

Reservoir fluids are mixtures consisting of a variety of hydrocarbon and non-hydrocarbon components. By nature, reservoir fluids have the ability to change their composition and make phase transitions under the influence of thermobaric conditions. In practice, such systems are characterized by three PVT parameters (Pressure – Volume – Temperature).

Reservoir oil fluids are complex mixtures of hydrocarbons, the composition and properties of which are unknown in detail. The light fraction of these liquids contains associated gases and low molecular weight hydrocarbons, for example: CO_2, H_2S, N_2, C_1, C_2, C_3, n-C_4, i-C_4, etc., while the rest of the oil contains a large amount of paraffin and naphthenic hydrocarbons, as well as aromatic compounds [1]. When modeling PVT properties of hydrocarbon systems, fractions above heptane are usually represented as a fraction of the residue – C_{7+}, and a generalized information about it is given (Fig. 1, *a*).

Typically, the behavior of reservoir fluids is described in the laboratory using integral functions such as volume coefficient, gas content coefficient, viscosity from pressure, density from pressure, etc. However, when we are dealing with volatile oils and gas condensates, where there is a mixture of several phases, integral functions are not able to describe the behavior of these mixtures. In this regard, the development and modeling, in such cases, requires a qualitative study of the composition of the mixture and an understanding of their phase transformations and physico-chemical properties when the mixture goes through the "formation – well – surface structure" path.

In practice, compositional modeling is used to describe the behavior of such mixtures. Compositional modeling implies that a detailed component composition will be used in the simulation, that is, the remainder of the positive heptane fraction will be divided into single components. It is worth noting that in practice, to speed up calculations, the components above the heptane fraction are grouped into pseudo-components (Fig. 1, *b*). As mentioned above, in this case, the data on the component composition become averaged and their application in modeling surface structures becomes difficult to apply. To model surface structures and the efficiency of field development, it is important to understand the detailed composition of the extracted products. To describe and obtain detailed data on the composition, in practice, the delumping process is used, which consists in dividing the C_{7+} residue into components (Fig. 2).
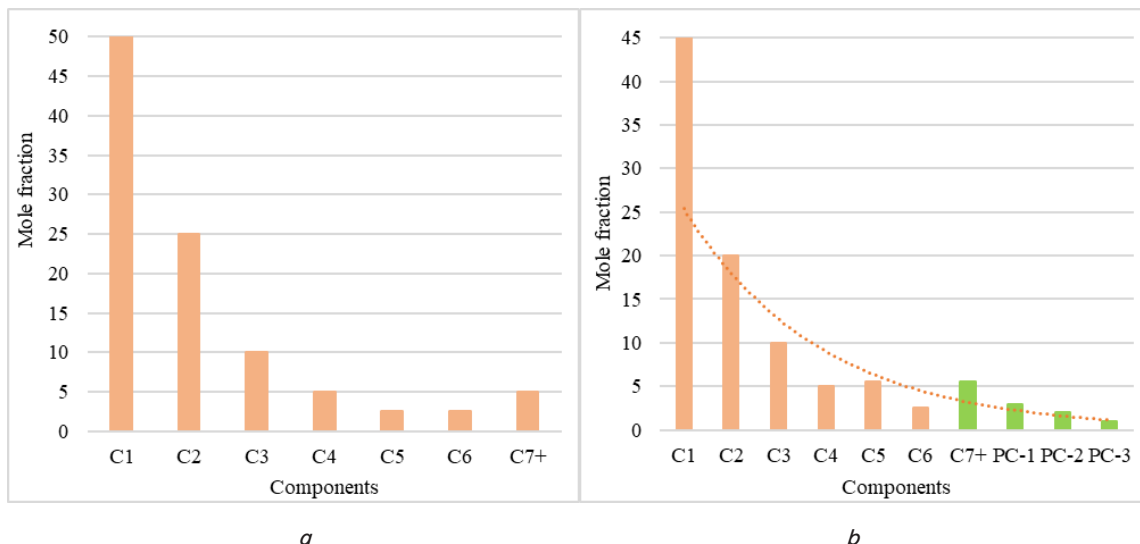
Fig. 1. Characteristics of the: a — fluid before the C_{7+} is divided into fractions; b — pseudo-components (PC-1, PC-2, PC-3) (the graphs are based on data from Tables 5, 6)
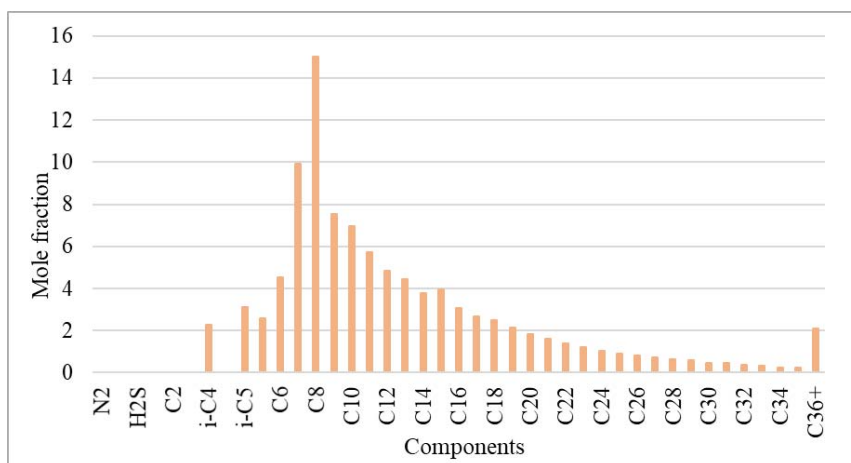

Fig. 2. Delumped system — characterized fluid (the graphs are based on data from Tables 5, 6)

Therefore, it is important to note that the availability of reliable information on the PVT properties of reservoir fluids plays an important role in the process of compositional modeling of both the formation and surface structures. In practice, the results of field, laboratory and theoretical studies are used to substantiate the properties of reservoir fluids. At each of these stages, engineers strive to obtain a reliable model and interpret it correctly.

Therefore, research devoted to the development of a delumping methodology in order to obtain a characterized fluid is relevant, since its results can have a significant impact on the modeling of oil surface structures.

2. Literature review and problem statement

Many works were devoted to the issues of compositional modeling, calculations of vapor-liquid equilibrium and adaptation of the PVT model. For example, in study [2] it is noted that three-parameter cubic equations of state are based on the component composition of a hydrocarbon system and have a large number of configurable parameters, the determination of

which, in laboratory conditions, becomes difficult. In this connection, there is a need to obtain additional data on the detailed component composition of the extracted products. Reservoir fluids, as a rule, can contain light and heavy fractions. Fractions being in different thermobaric conditions can be in different phase states. Light fractions with a low molecular weight are often in a gaseous state, while heavy fractions with a high molecular weight are in a liquid or solid state [1]. In study [1], the PVT model of gas condensate mixtures was adapted, but the cases of gas injection and determining the disequilibrium of phase transitions during field development were not considered.

In the study [3] mentioned that the set of necessary experimental data depends on the type of fluids and the very purposes of using the PVT model. However, the work did not fully disclose information that would give a clear idea of multicomponent mixtures. In the work [4] noted that the process of adapting the PVT model of multicomponent systems is complex and, in turn, requires an understanding of the thermodynamics of these systems. For a more detailed understanding, the authors proposed using the critical properties and the acentric factor of the individual components of the mixture. It is worth noting that, unlike the properties of

pure components, the properties of the fractions that make up natural hydrocarbon mixtures are not clearly defined. This is due to the fact that the fraction may include a different number of pure components in different ratios.

In production practice to adapt the PVT model by dividing the plus fraction into 4 pseudo-components, as mentioned earlier, in order to accelerate calculations of phase equilibrium. Later, [5] modified approach and proposed using a three-parameter equation of state, as well as adding critical parameters and an acentric factor for each component of the system. The accuracy of the approach is slightly reduced by non-zero BIP. Although the "detailed" EOS model was largely calibrated to data suitable for surface calculations, its accuracy under reservoir circumstances was not as good as it could be. In paper [6] proposed a new adaptation, but based on experimental data. Their approach was to split the remainder into fractions using a gamma-distribution model. It is worth noting that in all of the above approaches, the remainder of the heptane fraction (C_{7+}) is grouped into pseudofractions. However, one of the key drawbacks of this work is that the methodology requires a significant amount of initial data and experiments to fine tune the parameters of the equation of state. These disadvantages limit the widespread use of the method and make it less attractive for use in environments where data is limited or rapid assessment is required. It is also worth emphasizing that the study [7] notes the importance of using data on the molecular weight and specific gravity of the residue fraction C_{7+} for PVT reports and further modeling of the properties of a multicomponent mixture. Although new correlations have been developed in the article, they may not fully take into account the complexity of fluid behavior in reservoir conditions, especially for fluids that differ significantly from the average properties of the data set used.

As noted above, the process of delumping also plays an important role in compositional modeling. The delumping process helps to determine the detailed component composition of the system and gives a characteristic of each component. The issues of obtaining the characterized liquid published in research [8]. They created split parameters to associate the mixed components with the original components based on the composition of the oil, and used the equilibrium K-values for the mixed components to approximate the K-values for the original components. The equilibrium molar fractions of each detailed component were obtained using K-values for concentrated components and separation parameters, and these molar fractions were used to determine the phase characteristics of the concentrated model during the depletion process.

Similarly, [8] proposed a delumping procedure that determines phase equilibrium compositions at a certain pressure and temperature while maintaining thermodynamic consistency. When the binary interaction coefficients are zero, this method uses a linear relationship between the logarithm of the K-values and the EOS parameters. The ratio between K values and EOS parameters of pure components is defined specifically for standard EOS (such as Peng-Robinson or Soave-Redlich-Kwong).

Analytical methods can be used to determine the constants if all the coefficients of the binary interaction are zero. However, the equation becomes approximate when nonzero interactions are taken into account, and regression analysis is required to determine the constants. The LSK algorithm, developed by [9] includes an assessment of the equilibrium phase composition of a concentrated system under certain conditions to determine the values of K grouped components. Using either an analytical formula or the least squares method, ΔC are calculated for zero and non-zero binary interaction coefficients, respectively.

Taking into account the general detailed composition of the oil, then, based on these constants, the K-values for the initial components are set and used in the Rachford-Rice equation to calculate phase ratios and molar fractions of phases.

The research [10] developed an analytical solution that is equivalent even with non-zero binary interaction coefficients, and modified the LSK algorithm. They reformulated the EOS parameters and reduced the number of independent variables using a reduction strategy (reduction parameters). They then used the LSK algorithm with a new formulation to determine the ungrouped system at a certain pressure and temperature and were able to achieve surprisingly consistent results between the properties of the ungrouped compositions and the properties of the initial working fluid [10]. The ln(ki) ungrouping equation relates the equilibrium ratio of a complex solution to the consequences of instantaneous calculations (flash calculations) for a grouped liquid and extends to systems with non-zero binary interaction parameters.

The paper [11] compared analytical delumping, as described in [10], with LSK delumping [9] in the context of reservoir simulation results. The authors concluded that analytical delumping delivers more accurate and superior results compared to LSK delumping. The essence of this conclusion is that the first method uses BIP based on the reduction method.

Most of the above studies do not describe in detail the cases when gas is injected and the composition of the extracted products has more than one phase. All this allows to argue that it is appropriate to conduct a study devoted to developing a more cost-effective and practical method for parameter determination in PVT models, which would significantly enhance the accuracy and applicability of these models in industrial settings, in order to obtain a detailed liquid.

3. The aim and objectives of the study

The aim of the study is to modifying the method analysis method that allows to characterize the detailed composition of the petroleum fluid. This may be crucial in modeling reservoirs and surface oil facilities.

To achieve this aim, the following objectives are accomplished:

– to calculate the critical parameters and binary interaction parameters (BIP) for the PVT model;

– to calculate the reduction parameters for efficient processing of the parameters of the binary interaction of components;

– to perform a flash calculation to obtain a vapor-liquid equilibrium;

– to evaluate our proposed delumping method against the outcomes from PVTsim and laboratory analysis delumping.

4. Materials and methods

The object of the study is samples of Kazakhstani oil. The hypothesis of the study is to application of the delumping method will allow obtaining detailed fluid characteristics. In order to implement the study, oil samples were taken from the X field. The basic information about the deep-oil sample is presented in Table 1. It is worth noting that the component composition of the selected sample was analyzed experimentally by gas chromatography. The selected samples allowed to obtain representative data for evaluation and calculations.

Table 1

Properties of deep-oil sample from X field

Properties	Results
Reservoir pressure, MPa	37.92
Reservoir temperature, °C	129
Bubble point pressure, MPa	20.65
Z-factor at reservoir pressure	0.89
Oil density at standard condition, kg/m³	0.8021

The research used an integrated approach, including a combination of different methods, to ensure the accuracy and reliability of the results obtained. For example, the delumping of pseudo-components into single independent components was calculated on the basis of the Nichita-Leibovici analytical method and the LSK method with the use of zero parameters of binary interaction (BIP) for calculations of vapor-liquid equilibrium. It can be assumed that a detailed component composition can be obtained in more than one way.

Kazakhstani oils are characterized as highly viscous hydrocarbon components, mainly consisting of heavy residue fractions. Understanding the physical and chemical properties of such residues plays an important role in the development of deposits. The choice of the above methods lies in their reliability for the analysis of complex hydrocarbon systems. The Nichita-Leibovici and Leibovici-Stenby-Knudsen methods have important differences in their approaches and applications, although both aim to improve the accuracy of modeling hydrocarbon mixtures. The Nichita-Leibovici method focuses on setting non-zero BIPs for a wide range of mixtures, while the Leibovici-Stenby-Knudsen method, taking into account zero BIPs, focuses on delumping and detailed analysis of complex mixtures.

The critical parameters and the acentric factor of the components were calculated on the basis of the Lee-Kesler correlation, since experimental data were limited, and the availability of critical system data plays an essential role in compositional modeling. It is worth noting that all calculations were made under the assumption that two phases coexist in the mixture: liquid and vaporous.

5. Results of pressure-volume-temperature analysis using various methods of delumping

5. 1. Calculation of critical parameters and coefficients of binary interaction of a hydrocarbon system to create a pressure-volume-temperature model

Effective field development has a significant impact on the production process, and subsequently is important in the planning and modeling of refineries. In order to simulate the processes of oil recovery and design of ground structures, the engineer uses hydrodynamic models. One of the important parts of such models is the PVT model of reservoir hydrocarbon systems. The presence of such models makes it possible to clearly understand the composition of the products to be extracted, and also gives an idea of the phase state of the mixture.

In practice, engineers use a technique to characterize the PVT properties of reservoir fluids, which in turn is based on the application of cubic equations of state and calculations of vapor-liquid equilibrium.

In the oil industry, the most common equations of state are the Peng-Robinson and Soave-Redlich-Kwong equations of state. Models of such equations of state are based on the component composition of the hydrocarbon mixture. As part of the study, the results of which are displayed in this article, the Peng-Robinson equation of state is applied.

When creating a PVT model of hydrocarbon systems, the results of laboratory data from representative deep oil samples are required. The availability of experimental data on samples allows to build a model that adequately describes the properties of the mixture over a wide range of temperature and pressure parameters. In practice, in the laboratory, a detailed component composition is obtained using gas chromatography. The results of gas chromatography make it possible to divide the system into liquid and vapor phases. It is worth noting that in laboratory conditions, in most cases, the liquid phase is separated to C_{36+}, and the vapor phase to C_{10+}.

In PVT modeling of multicomponent systems using the Peng-Robinson equation of state, all parameters of the equation are required in order to calculate its coefficients. For the procedure of these calculations, it is important to set the correct molar fractions and critical properties of each component of the mixture, namely the critical temperature (Tc) and critical pressure (Pc), the acentric factor ω), as well as the binary interaction coefficients (k_{ij}), which in turn show the interaction between the components. Table 2 provides information on the critical parameters of the components calculated for the sample from X field.

Binary interaction parameters play an important role in the calculations of vapor-liquid equilibrium. These coefficients are correction factors in the mixing rules and are used when calculating the value of "a" in the equations of state. Table 3 shows the zero BIP's for the sample from field X.

The introduction of k_{ij} – binary interaction coefficients, significantly increases the accuracy of calculating the vapor-liquid equilibrium using the EOS.

Table 2

Critical parameters and acentric factors for sample from X field

Components		Tc **(K)**	Pc **(bar)**	Acentric factor, ω	Molecular weight, g/l
1	**2**	**3**	4	5	6
Nitrogen	**N₂**	**126.2**	33.94	0.040	28.014
Carbon dioxide	CO₂	304.2	73.76	0.225	44.01
Hydrogen sulfide	H₂S	497.4	1.991	0.285	34.08
Methane	C₁	576.1	1.949	0.067	16.043
Ethane	C₂	628.8	1.920	0.198	30.07
Propane	C₃	670.6	1.898	0.152	44.097
Isobutane	i-C₄	670.6	1.898	0.176	58.124
Butane	n-C₄	706.2	1.878	0.193	58.124

1	2	3	4	5	6
Isopentane	i-C5	706.2	1.878	0.227	72.151
Pentane	n-C_5	737.6	1.862	0.251	72.151
Hexane	C_6	765.9	1.846	0.296	86.178
Heptane	C_7	792.0	1.833	0.337	96
Octane	C_8	816.2	1.820	0.374	107
Noonan	C_9	838.9	1.808	0.421	121
Decane	C_{10}	860.3	1.796	0.482	134
Undecane	C_{11}	880.7	1.785	0.483	147
Dodecane	C_{12}	900.2	1.775	0.570	160.92
Tridecan	C_{13}	918.8	1.765	0.571	174.98
Tetradecan	C_{14}	936.7	1.755	0.660	187.93
Pentadecan	C_{15}	954.0	1.746	0.661	205.83
Hexadecane	C_{16}	970.7	1.737	0.750	220.12
Heptadecane	C_{17}	986.8	1.728	0.751	236.94
Octadecane	C_{18}	1002.5	1.720	0.828	250.96
Nonadecan	C_{19}	1017.8	1.711	0.829	262.99
Eicosane	C_{20}	1032.6	1.703	0.913	274.99
Geneicosane	C_{21}	1047.1	1.695	0.914	290.99
Docosane	C_{22}	1061.3	1.687	0.915	304.99
Triclosane	C_{23}	1075.1	1.679	1.035	317.99
Tetracosanee	C_{24}	1088.6	1.671	1.036	330.99
Pentacosane	C_{25}	1101.8	1.664	1.037	344.99
Hexacosan	C_{26}	1114.8	1.656	1.038	358.99
Heptacosane	C_{27}	1127.5	1.648	1.039	373.99
Octacosane	C_{28}	1140.0	1.641	1.181	387.99
Nonacosane	C_{29}	1152.3	1.634	1.182	401.99
Triacontane	C_{30}	1164.4	1.626	1.183	416
Gentriacontane	C_{31}	1176.3	1.619	1.184	430
Dotriacontane	C_{32}	1187.9	1.612	1.185	444
Tritriacontane	C_{33}	1199.4	1.604	1.185	458
Tetratriacontane	C_{34}	1210.8	1.597	1.151	472
Pentatriacontane	C_{35}	1221.9	1.590	1.151	486
Hexatriacontane plus	C_{36+}	1221.9	9.290	1.152	632.257

Table 3

Zero binary interaction parameters for X field

k_{ij}	N_2	CO_2	C_1	C_2	C_3	i-C_4	C_4	i-C_5	C_5	C_6	PC_1	PC_2	PC_3	PC_4
N_2	**0.0000**	0.0015	0.0023	0.0000	0.0015	0.0040	0.0040	0.0068	0.0068	0.0097	0.0268	0.0321	0.0295	0.0138
CO_2	0.0544	0.0000	0.0075	0.0011	0.0000	0.0006	0.0006	0.0019	0.0019	0.0036	0.0159	0.0201	0.0180	0.0063
C_1	0.0023	0.0075	0.0000	0.0029	0.0075	0.0123	0.0123	0.0169	0.0169	0.0212	0.0440	0.0505	0.0473	0.0271
C_2	0.0000	0.0011	0.0029	0.0000	0.0011	0.0033	0.0033	0.0059	0.0059	0.0086	0.0250	0.0301	0.0276	0.0125
C_3	0.0015	0.0000	0.0075	0.0011	0.0000	0.0006	0.0006	0.0019	0.0019	0.0036	0.0159	0.0200	0.0180	0.0063
i-C_4	0.0040	0.0006	0.0123	0.0033	0.0006	0.0000	0.0000	0.0004	0.0004	0.0013	0.0104	0.0138	0.0121	0.0030
C_4	0.0040	0.0006	0.0123	0.0033	0.0006	0.0000	0.0000	0.0004	0.0004	0.0013	0.0104	0.0138	0.0121	0.0030
i-C_5	0.0068	0.0019	0.0169	0.0059	0.0019	0.0004	0.0004	0.0000	0.0000	0.0003	0.0068	0.0097	0.0082	0.0013
C_5	0.0068	0.0019	0.0169	0.0059	0.0019	0.0004	0.0004	0.0000	0.0000	0.0003	0.0068	0.0097	0.0082	0.0013
C_6	0.0097	0.0036	0.0212	0.0086	0.0036	0.0013	0.0013	0.0003	0.0003	0.0000	0.0044	0.0068	0.0056	0.0004
PC_1	0.0268	0.0159	0.0440	0.0250	0.0159	0.0104	0.0104	0.0068	0.0068	0.0044	0.0000	0.0003	0.0001	0.0022
PC_2	0.0321	0.0201	0.0505	0.0301	0.0200	0.0138	0.0138	0.0097	0.0097	0.0068	0.0003	0.0000	0.0001	0.0040
PC_3	0.0295	0.0180	0.0473	0.0276	0.0180	0.0121	0.0121	0.0082	0.0082	0.0056	0.0001	0.0001	0.0000	0.0031
PC_4	0.0138	0.0063	0.0271	0.0125	0.0063	0.0030	0.0030	0.0013	0.0013	0.0004	0.0022	0.0040	0.0031	0.0000

5. 2. The results of the calculation of the reduction parameters in order to obtain a detailed liquid

The reduction method provides an effective analytical approach for handling non-zero binary interaction parameters. Nevertheless, as the mole fraction of a component increases, the BIP also increases, it was noted above. There-fore, for cases involving non-zero BIPs between pseudo-components, it is necessary to employ the analytical delumping approach proposed by [10]. This method utilizes a smaller range of reduction variables compared to the initial parameter range. The calculated reduction parameters derived from field data are presented in Table 4.

Table 4

Calculated reduction parameters for sample from X field

Liquid phase		Vapor phase	
Z_L	**0.845**	Z_V	**0.975**
E_L	**1.025**	E_V	**1.011**
λ_L	8.168	λ_V	1.781
θ_{kL}	1.633	θ_{kV}	1.115
A_L	0.128	A_V	0.028
B_L	0.0075	B_V	0.004
h_{0L}	0.177	h_{0V}	−0.028
$h_{\alpha L}$	**19.159**	$h_{\alpha V}$	**3.639**
h_{BL}	**−40.608**	h_{BV}	**−51.209**
$h_{\gamma kL}$	**3.829**	$h_{\gamma kV}$	**2.279**
Δh_0		**0.2059**	
Δh_α		**15.5192**	
Δh_B		**10.6012**	
$\Delta h_{\gamma k}$		**1.5500**	

Fig. 3 shows cross graph of the delumped $\ln(K)$ dependence on the $\ln(K)$ of the detailed.
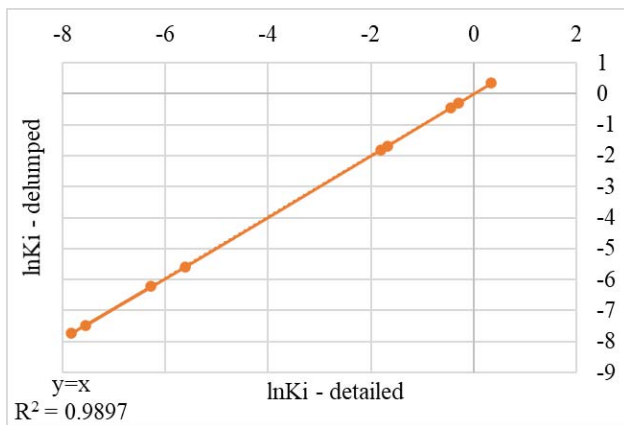

Fig. 3. Cross graph of ln(k) of the delumped and initial mixtures

The proposed method provides an excellent correspondence between the phase equilibrium constants and the molar fractions of the mixture components. It is important to note that there is a linear dependence ($y=x$) between the equilibrium constants for the detailed and delumped systems.

5. 3. The importance of calculating vapor-liquid equilibrium in compositional modeling

The fluid, being in reservoir conditions, can be in a single-phase state, however, when the process of raising it to the surface occurs, thermobaric changes can lead to the fact that the fluid can undergo various phase transitions and transition from a single-phase state to a two-phase one, because gas can begin to be released from oil.

The thermodynamic equilibrium between the vapor and liquid phases is expressed in terms of the equality of the volatility of the i-th component in the vapor phase and the volatility of the i-th component in the liquid phase, is written according to the following equality:

$$f_i^V = f_i^L, \tag{1}$$

where are f_i^V – volatility of the vapor phase and f_i^L – volatility of the liquid phase.

Schematically, it can be seen from Fig. 4 that flash calculation is a process during which the phase equilibrium of a mixture (Z_i) is determined at given pressure (P) and temperature (T) parameters.
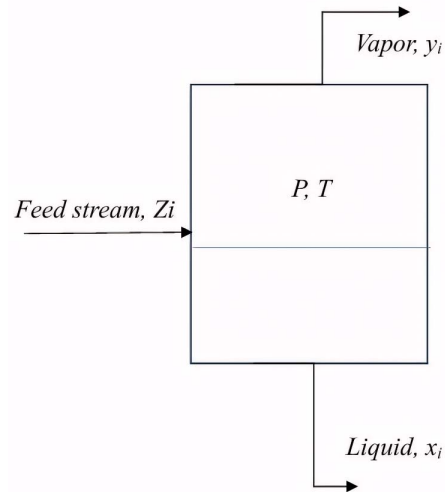

Fig. 4. An illustrative example of flash calculation

The calculation stages for determining y_i and x_i of a hydrocarbon mixture with a known total composition Z_i are characterized by a set of phase equilibrium constants K_i.

Therefore, the phase equilibrium constant is a dimensionless ratio of the molar fractions of a component in the gas phase to its molar fraction in the liquid phase in the presence of thermodynamic equilibrium between them, i. e.:

$$K_i = \frac{y_i}{x_i}. \tag{2}$$

The Rachford-Rice equation is used to calculate the vapor and liquid phases:

$$x_i = \frac{z_i}{1+V(K_i-1)},$$

and:

$$y_i = K_i x_i = \frac{z_i K_i}{1+V(K_i-1)}. \tag{3}$$

where K_i – phase equilibrium constant (K-value); x_i – liquid mole fraction, component i; y_i – vapor mole fraction, component i; V – the partial fraction of the vapor phase; Z_i – total composition.

Table 5 shows the results of the flash calculation calculated using the example of Kazakhstani oil.

It is worth noting that all calculations were made under the assumption that two phases coexist in the mixture: liquid and vaporous.

Table 5

Results of flash calculation of some components of the sample mixture of the Kazakhstani X field

Component	Flash of initial systems			Analytical delumped			Component	Flash of lumped systems		
	K_i	y_i	x_i	K_i	y_i	x_i		K_i	y_i	x_i
i-C$_4$	**1.411**	0.032	0.023	1.411	0.032	0.023	i-C$_4$	4.022	0.092	0.022
i-C$_5$	0.645	0.020	0.031	0.645	0.020	0.031	n-C$_4$	2.800	0.000	0.000
n-C$_5$	0.745	0.019	0.026	0.744	0.019	0.026	i-C$_5$	1.114	0.035	0.031
C$_6$	0.187	0.008	0.045	0.186	0.008	0.045	n-C$_5$	0.807	0.022	0.027
C$_7$	0.163	0.016	0.099	0.164	0.016	0.099	C$_6$	0.265	0.012	0.044
C$_8$	0.004	0.001	0.150	0.004	0.001	0.150	C$_7$–C$_{11}$	0.021	0.010	0.450
C$_9$	0.001	$3*10^{-5}$	0.075	0.001	$3*10^{-5}$	0.075				
C$_{10}$	0.002	0.0001	0.069	0.002	0.0001	0.069	C$_{12}$–C$_{19}$	0	0	0.273
C$_{11}$	0.001	$3*10^{-5}$	0.058	0.001	$3*10^{-5}$	0.058				

5. 4. Comparative analysis of proposed delumping with software simulation and experimental data

In order to confirm that the application of the analytical method for obtaining a detailed fluid can be of practical use, Table 6 shows the results of three evaluation methods: laboratory test, analytical method and software simulation.

Fig. 5 illustrates the phase boundaries of the mixture under investigation.

Analysis of this graph reveals a strong correlation between the phase boundaries for saturation pressure, with only minor and acceptable discrepancies observed for the dew points.

Table 6

Delumping results obtained from experimental test, proposed analytical method and PVTsim simulation

Components		Experimental test		PVTsim simulation		Proposed method	
		Liquid, mole %	Vapor, mole %	Liquid, mole %	Vapor, mole %	Liquid, mole %	Vapor, mole %
1	2	3	4	5	6	7	8
Nitrogen	N$_2$	0.818	1.174	0.8229	1.169	0.817	1.175
Carbon dioxide	CO$_2$	0.108	0.155	0.1090	0.150	0.108	0.155
Hydrogen sulfide	H$_2$S	0.000	0.000	0.000	0.000	0.000	0.000
Methane	C$_1$	46.474	66.758	46.752	66.215	47.672	66.749
Ethane	C$_2$	7.212	10.361	7.255	9.891	7.217	10.359
Propane	C$_3$	6.450	9.266	6.488	9.005	6.459	9.270
Isobutane	i-C$_4$	1.748	2.197	1.758	2.052	1.750	2.197
Butane	n-C$_4$	2.976	4.275	2.993	4.035	2.982	4.275
Isopentane	i-C5	1.734	1.518	1.7443	1.515	1.731	1.518
Pentane	n-C$_5$	1.955	1.489	1.9667	1.398	1.951	1.490
Hexane	C$_6$	2.573	0.903	2.5884	0.875	2.572	0.899
Heptane	C$_7$	3.185	1.803	3.2040	1.791	3.190	1.803
Octane	C$_8$	5.548	0.077	5.5812	0.077	5.542	0.077
Nonane	C$_9$	2.627	0.019	2.8559	0.018	2.628	0.019
Decane	C$_{10}$	2.200	0.005	1.7514	0.004	2.211	0.005
Undecane	C$_{11}$	1.741	0.001	2.7936	0.001	1.743	0.001
Dodecane	C$_{12}$	1.458	0.001	2.2554	0.000	1.443	0.001
Tridecane	C$_{13}$	1.319	–	2.3147	–	1.320	–
Tetradecane	C$_{14}$	1.135	–	1.1136	–	1.135	–
Pentadecane	C$_{15}$	1.107	–	1.5844	–	1.116	–
Hexadecane	C$_{16}$	0.856	–	1.2142	–	0.911	–
Heptadecane	C$_{17}$	0.749	–	0.8510	–	0.780	–
Octadecane	C$_{18}$	0.696	–	0.745	–	0.721	–
Nonadecane	C$_{19}$	0.59	–	0.682	–	0.636	–
Eicosane	C$_{20}$	0.517	–	0.619	–	0.568	–
Geneicosane	C$_{21}$	0.468	–	0.458	–	0.463	–
Docosane	C$_{22}$	0.407	–	0.499	–	0.453	–
Triclosane	C$_{23}$	0.383	–	0.483	–	0.433	–
Tetracosanee	C$_{24}$	0.317	–	0.315	–	0.316	–
Pentacosane	C$_{25}$	0.296	–	0.297	–	0.297	–
Hexacosane	C$_{26}$	0.263	–	0.261	–	0.262	–
Heptacosane	C$_{27}$	0.233	–	0.310	–	0.272	–
Octacosane	C$_{28}$	0.208	–	0.202	–	0.205	–
Nonacosane	C$_{29}$	0.207	–	0.183	–	0.195	–

Continuation of Table 6

1	2	3	4	5	6	7	8
Triacontane	C_{30}	0.18	–	0.131	–	0.156	–
Gentriacontane	C_{31}	0.177	–	0.159	–	0.168	–
Dotriacontane	C_{32}	0.143	–	0.150	–	0.147	–
Tritriacontane	C_{33}	0.142	–	0.124	–	0.133	–
Tetratriacontane	C_{34}	0.1	–	0.100	–	0.100	–
Pentatriacontane	C_{35}	0.104	–	0.106	–	0.105	–
Hexatriacontane plus	C_{36+}	0.567	–	0.571	–	0.569	–
Balance		100	100	100	100	100	100
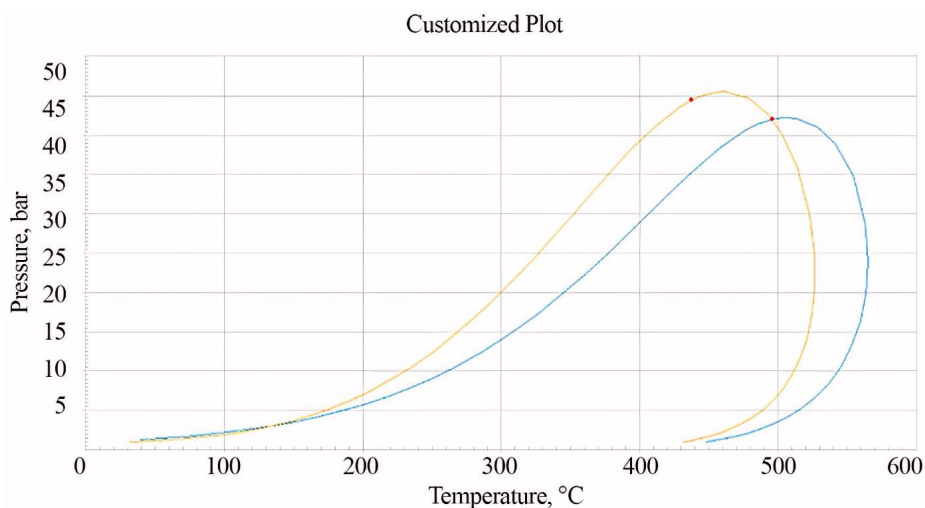
Fig. 5. Phase PT envelope for characterized and lumped fluid (blue line — lumped; yellow line — characterized; red point — critical points)

6. Discussion of the received delumping results

Delumping in hydrocarbon compositional modeling refers to the process of breaking down aggregated pseudo-components into their individual constituent components. This technique is used to achieve more accurate and detailed compositional simulations in reservoir engineering and production forecasting.

Understanding the detailed composition of the fluid helps to effectively plan not only the development of the field, but also the modeling of ground structures, where the phase behavior of the mixture plays an essential role. Adapting the customized PVT model of the hydrocarbon system helps to make different predictions, in the sense that based on the customized PVT model, it is possible to optimize the surface collection system, modeling surface structures and can consider cases of gas injection and assess in which cases the gas will mix or not and evaluate the effect of this injection.

From the analysis of existing literature, it can be noted that the paper [9] emphasizes the enhanced accuracy of the compositional delumping method, particularly in cases with non-zero BIP. When comparing the LSK method [9] with the analytical delumping approach [10], it was consistently found that analytical delumping yields better results than LSK delumping.

As part of the research described in this article, the delumping of the composite modeling results were conducted using analytical approach with BIP and reduction parameters. The quality of delumping depends on lumping and their consistency is important because of the usage of the same EOS parameters. The flash calculations which based on analytical delumping

method which uses Rachford-Rice equation is more efficient than equations embedded in simulation programs. Subsequently the data may be utilized to successfully determine the detailed composition from a pseudo-component.

This research establishes a connection with the work presented in [10], where an enhancement to the LSK approach was introduced along with an innovative analytical reduction based on delumping technique. Notably, this approach demonstrated efficacy in managing scenarios characterized by binary interaction coefficients. This work is aligned with the overarching objective of mitigating the challenges posed by zero BIP's through the application of analytical delumping, underscoring its importance over regression-based methodologies. Using the critical parameters presented in Table 2 and the BIP in Table 3, the reduction parameters were estimated for each phase, which are presented in Table 4. Referring to the results obtained in this study, it can be noted that Tables 5, 6 show data on the delumping methodology, where the trend of changes in the molar fractions of components depending on the amount of carbon is clearly visible. For example, as the amount of carbon increases, the proportion of gas phase in the mixture decreases, and the proportion of the liquid phase increases.

Additionally, it's important to acknowledge a disadvantage, the use of numerical modeling tools like PVTsim is inherently based on specific assumptions and equations of state. Any differences between these assumptions and actual conditions can impact the accuracy of the results.

However, this study has limitations in the form of the fact that the input data for calculations were taken for sam-

ples of one specific region, in our case, Kazakhstani oil. But despite this, it is possible to obtain improved results of the delumping method, which have excellent consistency with the results of the PVTsim simulation, which indicates the applicability of the model.

Future development should aim to expand the input data for a wider range of oil samples and their testing, in order to possibly create a reference algorithm for the delumping model that could be applied to all possible cases.

7. Conclusions

1. Each independent component of the oil mixture has its own critical properties. The presence of such properties helps to understand more precisely at what thermobaric properties the component will begin to be in thermobaric equilibrium. Binary interaction parameters play an important role in the calculations of vapor-liquid equilibrium. These coefficients are correction factors in the mixing rules and are used when calculating the value of "a" in the equations of state.

2. The practical application of reduction parameters is to divide pseudo-components into independent components. These methods help to reconstruct the phase and component distribution of the characterized mixture using information on flash calculations of the grouped mixture. The basic concept of reduction parameter is to express the volatility coefficients as a function of a reduced number of variables. It is important to note that the reduction method becomes more effective with an increase in the number of components and a decrease in the number of non-zero binary interaction coefficients (BIP).

3. Understanding the phase behavior of multicomponent mixtures plays an essential role in compositional modeling. The presence of coexisting phases of the system gives a clear understanding of the state in which one or another component of the system will be in various thermobaric conditions. In practice, calculations of vapor-liquid equilibrium or calculation of an isothermal flash give the results of molar fractions in the general system. From obtained results, the natural logarithm of volatility has negative values and tend to decrease with increasing number of carbon atoms, thereby potentially expanding the liquid phase.

4. The proposed method of delumping has the closest values to experimental data. The simulation in PVTsim software has some deviations below 5 %, this is due to the fact that the Rachford-Rice equation is not used in the simulation, which is not included in the series of equations of the program.

Conflict of interest

The authors declare that they have no conflicts of interest in relation to the current study, including financial, personal, authorship, or any other, that could affect the study and the results reported in this paper.

Financing

Data availability

Data will be made available on reasonable request.

Use of artificial intelligence

The authors confirm that they did not use artificial intelligence technologies when creating the current work.

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