

The Delumping Method as a Key Factor in obtaining a characterized Hydrocarbon Fluid using the Example of Kazakhstani Oil

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ABSTRACT

The composition of hydrocarbon systems plays an essential role in ensuring reliability in field operation processes, the design of oil onshore facilities, and the availability of reliable information about the PVT properties of systems. In this article, experimental and numerical methods are used to obtain data on the component composition of the extracted oil products and their PVT properties. These methods help obtaining a detailed composition and phase state of the hydrocarbon system. The numerical delumping method is utilized in this article. It is worth noting that all calculations were made on the basis of data on the component composition of Kazakhstani oil samples. The results and comparative evaluation show that the proposed delumping mix-method has excellent consistency with the data obtained with experiments and with the Nichita's analytical approach. In the future, the results on the detailed composition can improve and link the compositional modeling of the reservoir with the modeling of surface structures.

Keywords-delumping; phase behavior; compositional modeling; pseudo-components; K-value

I. INTRODUCTION

Hydrodynamic models play a crucial role in the design and management of oil and gas field development in the petroleum industry. Oil and gas fields are reservoirs containing hydrocarbon compounds, which are complex multicomponent mixtures. The individual substances that make up these mixtures are referred to as the components of the mixture. Many hydrodynamic models have been proposed, with the PVT model of reservoir hydrocarbon mixtures being one of the most important [1, 2]. The construction of the PVT model consists in a technique that includes the use of three-parameter cubic equations of state and modeling of vapor-liquid equilibrium of multicomponent mixtures [3]. It is worth noting that the most common equations of state of these models are the Peng-Robinson and Soave-Redlich-Kwong equations [4]. The application of cubic equations of state is based on the composition of the produced well products, whereas these equations also include a sufficient number of configurable parameters. It is important to emphasize that these parameters are difficult to determine in the laboratory, but their application is widely used to the PVT model [5]. Authors in [2, 6] mention that the improvement of the PVT model requires laboratory data results, which in turn can be obtained from representative samples, and the set of required laboratory data depends on the type of liquid. Since it has already been emphasized that the equations of state are an important part of adaptation and require adjustments, authors in [7] were the first to propose a tuning algorithm. The essence of their proposal was that they recommended splitting the heavy residue of the heptane-plus (C7+) fraction into 4 pseudo-components and varying the parameters of the binary interaction between methane and each pseudo-component. Authors in [2] recommended using the setting utilizing critical parameters of independent fractions. This approach was further modified and the remainder was divided into pseudo-components with the gamma distribution method, critical parameters were calculated using correlation, and the acentric factor parameter was proposed in [8].

The procedure of grouping the fraction of the remainder into pseudo-components is called lumping. It is worth noting that this procedure is conducted in order to reduce the calculation time, since the process of compositional modeling of the reservoir and well requires a large number of phase equilibrium calculations [9, 10]. However, when the extracted fluid gets to the surface, it is important to understand the detailed composition of the hydrocarbon mixture, because in

each model, the fluid will vary. It will be one extracted product, but the number and composition of its components in the reservoir model will differ from that in the surface model.

Since the results obtained in the lumping process give only an average value of the fraction of the residue (C7+), for modeling surface objects, it is necessary to ungroup pseudo-components into single independent components [11]. The ungrouping procedure, in practice called delumping, allows engineers to ensure the compositional behavior of the characterized liquid for the purposes of not only planning, but also modeling of oil and gas onshore structures. It is important to emphasize that component characterization means obtaining data on the molar fraction of each component and its phase state during the extraction process. The operation process is accompanied by phase transitions of components under the influence of various thermobaric conditions. In this regard, in order to ensure high-quality prediction of hydrocarbon production levels, taking into account the volume of each phase, a reliable assessment of the distribution of components of the hydrocarbon system between the liquid and vapor phases is necessary when their thermobaric conditions change [12].

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. Authors in [13, 14] drew attention to the issues of obtaining the characterized liquid. 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 of the original components. The equilibrium molar fractions of each detailed component were obtained using the 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.

Authors in [5] 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 [9, 19]. The $\ln(K_i)$ delumping equation relates the equilibrium ratio of a complex solution to the consequences of flash calculations for a grouped liquid and extends to systems with non-zero binary interaction parameters.

II. MATERIALS AND METHODS

It was noted above that for correct modeling of PVT properties, experimental data from representative oil samples are required. As such data, in this research, the results of oil samples taken from the Kazakhstani X field were used. The main parameters of the sample are shown in Table I.

TABLE I. GENERAL INFORMATION OF OIL SAMPLE

Parameter	Value
Sample type	bottom-hole oil
Reservoir pressure, kgf/cm ²	53.8
Reservoir temperature, °C	30.2
Oil density at reservoir condition, g/cm ³	0.818
Oil viscosity at reservoir condition, cP	3.178

The selected oil sample, under standard conditions, was determined numerically using the gas chromatography method based on the results of laboratory studies of the liquid and vapor phases. The liquid phase was determined to the hexatriacontane component (C36+), and the vapor phase to the dean (C10). It is important to note that usually the component composition is determined using gas chromatography in molar fractions. To obtain the composition in molar fractions, in the framework of this research, the molecular weight of each component was used and the corresponding value was calculated with:

$$Z_i = \frac{w_i}{M_i} \quad (1)$$

$$\sum_{j=1}^N \frac{w_j}{M_j}$$

where Z_i is the molar fraction, w_i is the mole fraction, and M_i is the molecular weight of the i -th component of the system.

As part of the research described in this article, the approach of scientists Nichita and Leibovici is considered [2, 6]. The authors propose an analytical delumping method for EOS with binary interaction coefficients. The approach is based on the calculation of phase equilibrium constants, K -value, based on reduction parameters (Δ_h):

$$\ln K_i(Q_L, Q_V) = \Delta h_0(Q_L, Q_V) + \Delta h_\alpha(Q_L, Q_V)\alpha_i + \Delta h_\beta(Q_L, Q_V)B_i + \sum_{k=1}^m \Delta h_{\gamma k}(Q_L, Q_V)\gamma_{ki} \quad (2)$$

$$i = 1, nc$$

where the reduction parameters are proposed to be calculated with:

$$\Delta h_0 = h_{0L} - h_{0V} = -\ln(Z_L - B_L) + \ln(Z_V - B_V)$$

$$\Delta h_\alpha = h_{\alpha L} - h_{\alpha V} = \frac{2}{\Delta} \left(\frac{\lambda_V^{(i)}}{B_V} \ln E_V - \frac{\lambda_L^{(i)}}{B_L} \ln E_L \right)$$

$$\Delta h_B = h_{BL} - h_{BV} = \frac{Z_L - 1}{B_L} - \frac{Z_V - 1}{B_V} - \frac{1}{2} \left(\frac{h_{\alpha L} A_L}{\lambda_L^{(i)} B_L} - \frac{h_{\alpha V} A_V}{\lambda_V^{(i)} B_V} \right)$$

$$\Delta h_{\gamma k} = h_{\gamma kL} - h_{\gamma kV} \quad (3)$$

where Q is the vector of reduction parameter, L and V represent liquid and vapor states, and h is the reduction parameter function.

Next, using the flash calculation algorithm, the proportion of each phase present in the mixture is calculated under specified thermobaric conditions. When calculating flash, it is worth adhering to the following equality:

$$L + V = 1 \quad (4)$$

When studying the computational methods underlying the determination of the phase state of hydrocarbon systems, it is possible to use the well-known Rachford-Rice concentration equations for liquid (L) and vapor (V) phases:

$$x_i = \frac{z_i}{1 + V(K_i - 1)} \quad (5)$$

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

It is worth noting that when calculating the vapor-liquid equilibrium using the cubic equation of state of hydrocarbon mixtures, it is necessary to take into account the fact that such mixtures are multicomponent and the equation coefficients are determined by the properties of the components forming the hydrocarbon mixture and the fractions of each phase in the mixture. In reality, the vapor and liquid phases obey Raoul's law, because the phase equilibrium constants depend not only on thermobaric conditions, but also on the composition of each component, and therefore it is important to know the critical properties of each component forming the mixture. In this regard, in our theoretical model, we took into account the correction for the phase equilibrium constant using the Wilson approach, which is calculated according to:

$$K_i = \frac{P_{ci}}{p} \times \exp \left(5.37 \times (1 + \omega_i) \times \left[1 - \frac{T_{ci}}{T} \right] \right) \quad (6)$$

where P_{ci} is the critical pressure, T_{ci} is the critical temperature, T is the system temperature, P is the system pressure, and ω is the acentric factor. Equation (6) refers to an iterative method for predicting the value of the phase equilibrium constant. The iterative method is based on equations of state and has a setting for the parameters of the binary interaction between the components of the mixture.

III. RESULTS AND DISCUSSION

Using (1)-(6) and the statements described in the Materials and Methods section, it was possible to obtain data on the component composition of the hydrocarbon mixture using several approaches. The results are shown in Table II.

TABLE II. DELUMPING RESULTS OBTAINED FROM VARIOUS METHODS

Components		Experimental approach		Nichita's approach		Proposed mix-approach	
		Liquid, mole %	Vapor, mole %	Liquid, mole %	Vapor, mole %	Liquid, mole %	Vapor, mole %
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
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-C ₅	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
Nonan	C ₉	2.627	0.019	2.8559	0.018	2.628	0.019
Dean	C ₁₀	2.200	0.005	1.7514	0.004	2.211	0.005
Undecane	C ₁₁	1.741		2.7936	0.001	1.743	0.001
Dodecan	C ₁₂	1.458		2.2554	0.000	1.443	0.001
Tridecan	C ₁₃	1.319		2.3147		1.320	
Tetradecan	C ₁₄	1.135		1.1136		1.135	
Pentadecan	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	
Nonadecan	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	
Tricosane	C ₂₃	0.383		0.483		0.433	
Tetracosane	C ₂₄	0.317		0.315		0.316	
Pentacosane	C ₂₅	0.296		0.297		0.297	
Hexacosan	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	
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	
Triatriacontane	C ₃₃	0.142		0.124		0.133	
Tetraatriacontane	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	100

TABLE III. DATA OF FLASH CALCULATION OF SOME COMPONENTS OF THE OIL MIXTURE OF THE KAZAKHSTANI X FIELD

Component	Initial systems			Proposed delumping			Component	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

It can be seen that the sample under study mainly consisted of a methane fraction and all calculations were made based on the considerations that both phases coexist in the mixture. Understanding the phase behavior of multicomponent mixtures is crucial in compositional modeling. The coexistence of different phases within a system provides valuable insights into

the state of each component under varying thermobaric conditions. In practice, vapor-liquid equilibrium calculations or isothermal flash calculations yield the molar fractions of components within the overall system. Table III demonstrates the results of the flash calculation. The results typically show that the natural logarithm of volatility exhibits negative values

and decreases as the number of carbon atoms increases, which may contribute to the expansion of the liquid phase. For an illustrative example, based on the data given in Table II, diagrams of the mole fractions of the vapor and liquid phases, depending on the components, were constructed for all three possible methods of obtaining the characterized fluid illustrated and are shown in Figure 1.

Following the execution of calculations and the analysis of the results, it becomes evident that compositional modeling is a fundamental component in simulating the phase behavior and

properties of hydrocarbon systems, which are dependent on the detailed composition of the petroleum fluid. This modeling approach considers the phase equilibrium between coexisting phases, ensuring the maintenance of system balance. The outcomes of compositional modeling have practical applications not only in PVT analysis but also in enhanced oil recovery (EOR) techniques. In EOR methods, compositional models are employed to simulate CO₂ injection processes, providing insight into the miscibility of injected gases with reservoir fluids.

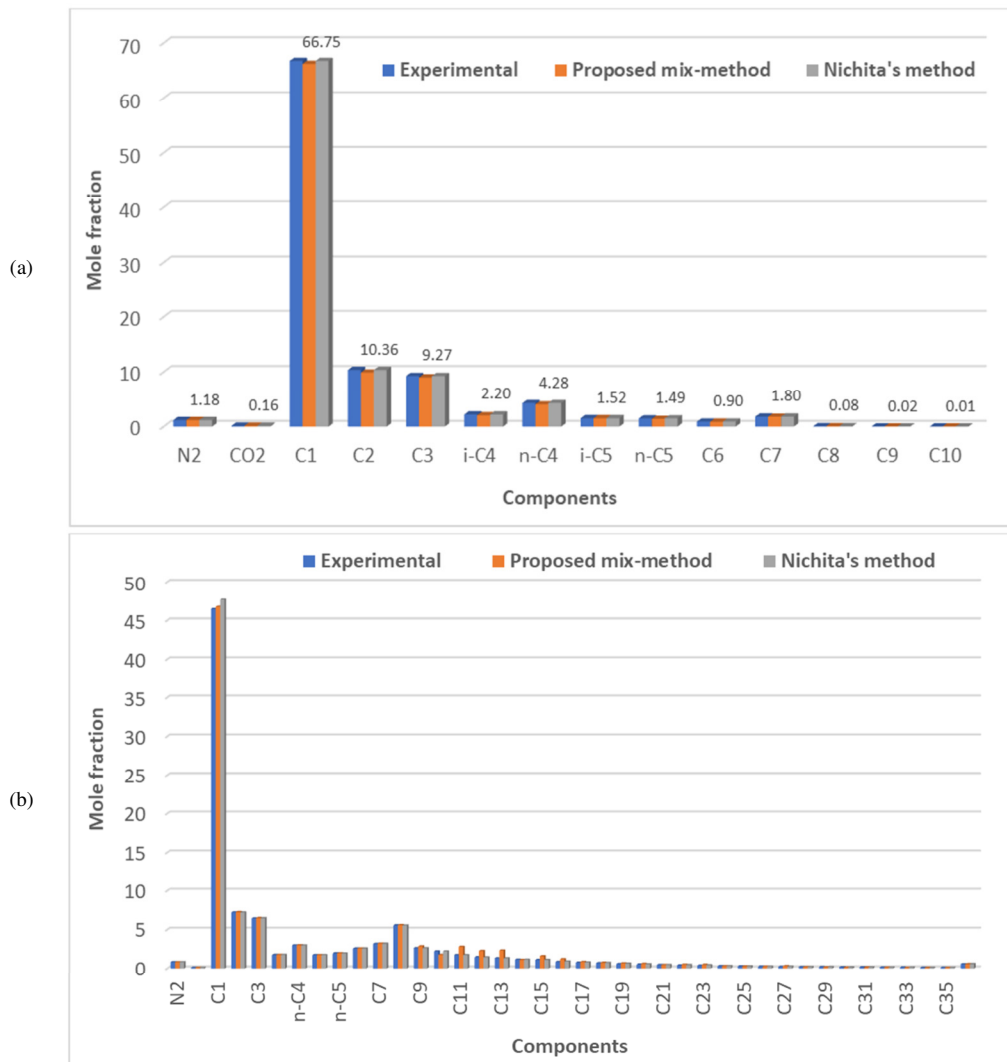


Fig. 1. Comparative diagram of the mole fraction of the delumped fluid system for: (a) vapor phase, (b) liquid phase.

IV. CONCLUSION

The current article considers an approach to the delumping of pseudo-components into independent real components. The computational aspect of the study was based on the analytical method of Nichita's delumping and the theoretical model proposed in this paper. The novelty of the study lies in the fact that the theoretical model described in this article took into account the correction for the phase equilibrium constant, since

during the production process it is important to pay attention to the phase state of the extracted fluid. A comparative analysis revealed that the method with correction closely aligns with the experimental data. The comparative evaluation confirms that delumping is a highly effective technique, offering a detailed understanding of the individual components present in extracted oil products and the phase transitions that occur during extraction and processing.

The delumping algorithm proves to be particularly valuable for reservoir and distillation process modeling, where precise knowledge of phase composition is critical. It is important to emphasize that the reliability and accuracy of PVT liquid model calculations using the equation of state are contingent not only on the quality and quantity of initial data regarding fluid composition and properties but also on the accuracy of phase behavior results.

Delumping techniques can be integrated with other methods, such as numerical evaluation and experimental measurements, to yield a comprehensive understanding of fluid behavior. The study's outcomes offer significant insights for reservoir engineers, researchers, and software developers in the domain of hydrocarbon reservoir modeling, enabling improved decision-making and more efficient operation. Therefore, researches devoted to the development of delumping methodology in order to obtain a characterized fluid are relevant, since they make a significant contribution to the modeling of refineries.

NOMENCLATURE

P	Pressure, MPa
T	Temperature, K
P_c	Critical pressure, MPa
T_c	Critical temperature, K
ω	Acentric factor
x_i	Liquid mole fraction, component i
y_i	Vapor mole fraction, component i
M	Molecular weight
GC	Gas chromatograph
EoS	Equation of state
BIP	Binary interaction parameters
V	Partial fraction of the vapor phase
L	Partial fraction of the liquid phase
K_i	Phase equilibrium constant (K-value)
Δh	Nichita's reduction parameters
Q	Vector of reduction parameters in Nichita's equation.
a_i	Reduction parameter in Nichita-Leibovici equation.
B_i	Reduction parameter in Nichita-Leibovici equation.
y_{ik}	Reduction parameter in Nichita-Leibovici equation.

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REFERENCES

- [1] T. S. Yushchenko and A. I. Brusilovsky, "A step-by-step approach to the creation and adaptation of PVT models of reservoir hydrocarbon systems based on the equation of state," *Georesursy*, vol. 24, no. 3, pp. 164–181, Apr. 2024, <https://doi.org/10.18599/grs.2022.3.14>.
- [2] C. H. Whitson and M. R. Brule, *Phase Behavior*. Richardson, TX, USA: Society of Petroleum Engineers, 2000.
- [3] C. F. Leibovici, J. W. Barker, and D. Wache, "Method for Delumping the Results of Compositional Reservoir Simulation," *SPE Journal*, vol. 5, no. 02, pp. 227–235, Jun. 2000, <https://doi.org/10.2118/64001-PA>.
- [4] B. Hussain and M. Ahsan, "A Numerical Comparison of Soave Redlich Kwong and Peng-Robinson Equations of State for Predicting Hydrocarbons' Thermodynamic Properties," *Engineering, Technology & Applied Science Research*, vol. 8, no. 1, pp. 2422–2426, Feb. 2018, <https://doi.org/10.48084/etasr.1644>.
- [5] R. C. Merrill, K. J. Hartman, and J. L. Creek, "A Comparison of Equation of State Tuning Methods," in *SPE Annual Technical*

Conference and Exhibition, New Orleans, LA, USA, Sep. 1994, <https://doi.org/10.2118/28589-MS>.

- [6] W. McCain, *Properties of Petroleum Fluids*, 3rd Edition. Tulsa, OK, USA: PennWell, 2017.
- [7] K. H. Coats and G. T. Smart, "Application of a Regression-Based EOS PVT Program to Laboratory Data," *SPE Reservoir Engineering*, vol. 1, no. 3, pp. 277–299, May 1986, <https://doi.org/10.2118/11197-PA>.
- [8] M. Assareh, C. Ghotbi, M. R. Pishvaie, and G. M. Mittermeir, "An analytical delumping methodology for PC-SAFT with application to reservoir fluids," *Fluid Phase Equilibria*, vol. 339, pp. 40–51, Feb. 2013, <https://doi.org/10.1016/j.fluid.2012.11.025>.
- [9] D. V. Nichita, D. Broseta, and C. F. Leibovici, "Reservoir fluid applications of a pseudo-component delumping new analytical procedure," *Journal of Petroleum Science and Engineering*, vol. 59, no. 1, pp. 59–72, Oct. 2007, <https://doi.org/10.1016/j.petrol.2007.03.003>.
- [10] M. Petitfrere and D. V. Nichita, "A comparison of conventional and reduction approaches for phase equilibrium calculations," *Fluid Phase Equilibria*, vol. 386, pp. 30–46, Jan. 2015, <https://doi.org/10.1016/j.fluid.2014.11.017>.
- [11] J. W. Barker and C. F. Leibovici, "Delumping Compositional Reservoir Simulation Results: Theory and Applications," in *SPE Reservoir Simulation Symposium*, Houston, TX, USA, Feb. 1999, <https://doi.org/10.2118/51896-MS>.
- [12] M. F. Hoda *et al.*, "Successful Implementations of Integrated Asset Modeling," in *SPE Intelligent Oil and Gas Symposium*, Abu Dhabi, United Arab Emirates, Dec. 2017, <https://doi.org/10.2118/187471-MS>.
- [13] A. G. Schlijper and J. K. Drohm, "Inverse Lumping: Estimating Compositional Data From Lumped Information," *SPE Reservoir Engineering*, vol. 3, no. 3, pp. 1083–1089, Aug. 1988, <https://doi.org/10.2118/14267-PA>.
- [14] A. Danesh, D. Xu, and A. C. Todd, "A Grouping Method To Optimize Oil Description for Compositional Simulation of Gas-Injection Processes," *SPE Reservoir Engineering*, vol. 7, no. 3, pp. 343–348, Aug. 1992, <https://doi.org/10.2118/20745-PA>.
- [15] C. Leibovici, E. H. Stenby, and K. Knudsen, "A consistent procedure for pseudo-component delumping," *Fluid Phase Equilibria*, vol. 117, no. 1, pp. 225–232, Mar. 1996, [https://doi.org/10.1016/0378-3812\(95\)02957-5](https://doi.org/10.1016/0378-3812(95)02957-5).
- [16] D. T. D. Castro, D. V. Nichita, D. Broseta, M. Herriou, and J. W. Barker, "Improved Delumping of Compositional Simulation Results," *Petroleum Science and Technology*, vol. 29, no. 1, pp. 1–12, Jan. 2011, <https://doi.org/10.1080/10916460903330098>.