

Simulation of composition changes in reservoirs with large hydrocarbon columns and temperature gradient

A.V. Yashin^{1,2*}, I.M. Indrupskiy^{1,2}, O.A. Lobanova¹

¹Oil and Gas Research Institute of the Russian Academy of Sciences, Moscow, Russian Federation

²Gubkin Russian State University of Oil and Gas (National Research University), Moscow, Russian Federation

Abstract. This paper compares three methods for calculation of initial composition variation with depth in hydrocarbon reservoirs: considering thermal diffusion, considering temperature gradient without thermal diffusion effects; and by gravity forces only. Newton method-based numerical algorithm was implemented for solution of thermodynamic equations to evaluate pressure and hydrocarbon composition. Test calculations are performed for main gas-condensate reservoir of Vuktylskoye field with a gas column of 1350 m.

The results obtained with the numerical algorithm indicate that gravity segregation impact is the strongest for all the cases considered. Concentration decreases with depth for low molecular weight components and increases for high molecular weight components. The higher molecular weight of the component, the stronger variation of its concentration with depth. Initial reservoir pressure also changes accordingly.

However, thermal diffusion also has a significant influence on variation of hydrocarbon composition with depth and initial reservoir pressure. For the test case considered, thermal diffusion magnifies the impact of gravity and results in strongly nonlinear dependencies of component concentrations on depth. When thermal gradient is taken into account without thermal diffusion effects, the results are only slightly different from those with the isothermal gravity segregation calculations.

None of the calculation methods were successful in matching estimates of initial composition variation with depth obtained from well exploitation data. Physical mechanisms governing variation of composition within the main reservoir of the Vuktylskoye field require additional investigation. Despite the long history of the reservoir development, this problem was previously studied based only on field development data.

Keywords: hydrocarbon mixture, geothermal gradient, thermal diffusion, component composition, initial composition, gas condensate reservoir, Vuktylskoye field

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Introduction

Hydrocarbon reservoirs with large oil or gas columns are characterized by significant changes in reservoir pressure and temperature with depth. As a result, the initial composition of the reservoir fluid also changes significantly with depth.

The distribution of components in depth in massive hydrocarbon reservoirs is greatly influenced by gravitational forces. Initial composition of the fluid in such reservoirs is formed in such a way that the concentration of light components decreases in the direction from the top to the bottom, while concentration of heavy components increases on the contrary. Accordingly, the content of

condensate in the reservoir gas increases and the solution-gas content in oil decreases.

In 1954, A.Y. Namiot made calculations for mixtures modeling oils of different composition (Namiot, 1954). It was concluded that gravity forces have a significant impact on the composition of oils containing significant amounts of heavy hydrocarbons and dissolved gas. In case of reservoirs consisting mainly of light hydrocarbons, the composition varies slightly with depth. Subsequently, the mathematical apparatus for calculating changes in multicomponent mixtures composition under the influence of gravity has been widely developed and applied (Whitson, Belery, 1994; Brusilovskii, 2002).

The method of calculating gravitational distribution of pressure and composition by reservoir depth is based on the assumption of the system thermodynamic equilibrium in the gravity field. This state of the system can be achieved at a constant system temperature throughout the entire volume.

*Corresponding author: Anton V. Yashin
E-mail: antn-yashin@yandex.ru

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Successive approximation of the variables is performed by solving at each step the system of equations $JS=F$ obtained by linearizing the equations of system (6). The matrix J and the vectors S, F have the following form:

$$J = \begin{pmatrix} \frac{\partial \Phi_1}{\partial p} & \frac{\partial \Phi_1}{\partial y_2} & \dots & \frac{\partial \Phi_1}{\partial y_N} \\ \dots & \dots & \dots & \dots \\ \frac{\partial \Phi_N}{\partial p} & \frac{\partial \Phi_N}{\partial y_2} & \dots & \frac{\partial \Phi_N}{\partial y_N} \end{pmatrix}; \quad S = \begin{pmatrix} p^{m+1} - p^m \\ y_2^{m+1} - y_2^m \\ \dots \\ y_N^{m+1} - y_N^m \end{pmatrix};$$

$$F = \begin{pmatrix} -\Phi_1^m \\ -\Phi_2^m \\ \dots \\ -\Phi_N^m \end{pmatrix} \quad (7)$$

where $m = 0, 1, 2, \dots$ is the iteration number.

The components of the matrix J are calculated as follows:

$$\frac{\partial \Phi_i}{\partial p} = \frac{\partial \ln f_i}{\partial p}, \quad i = 1, \dots, N; \quad (8)$$

$$\frac{\partial \Phi_i}{\partial y_j} = \frac{\partial \ln f_i}{\partial y_j} - \frac{\partial \ln f_i}{\partial y_1}, \quad i = 1, \dots, N, j = 2, \dots, N. \quad (9)$$

The apparatus of cubic equations of state is used for calculation of fugacities and their derivatives (Brusilovskii, 2002).

Within the approximate approach, it is possible to take into account temperature changes with depth in the system (4). For this, hydrocarbon column is divided into a number of small intervals and the temperature is considered constant within each interval. The difference in temperatures between the intervals should be taken into account when calculating fugacities; however, thermodynamic equilibrium conditions (1) are considered approximately valid. However, such a calculation neglects the heat transfer and the accompanying mass transfer of components caused by thermal diffusion.

Equation of state

The following Peng-Robinson cubic equation of state was applied to calculate the fugacities in this work:

$$Z^3 - (1 - B)Z^2 + (A - 3B^2)Z - (AB - B^2 - B^3) = 0. \quad (10)$$

For a given equation of state, the fugacities are calculated by the following formula:

$$\ln f_i = \ln(y_i p) + \frac{B_i}{B}(Z - 1) - \ln(Z - B) + \frac{A}{2\sqrt{2}B} \left(\frac{B_i}{B} - \frac{2}{A} \sum_{j=1}^N y_j A_{ij} \right) \ln \left[\frac{Z + (1 + \sqrt{2})B}{Z + (1 - \sqrt{2})B} \right], \quad (11)$$

where

$$Z = \frac{pv}{RT}, \quad (12)$$

$$A = \sum_{i=1}^N \sum_{j=1}^N y_i y_j A_{ij}, \quad (13)$$

$$B = \sum_{i=1}^N y_i B_i, \quad (14)$$

$$A_{ij} = (1 - k_{ij}) \sqrt{A_i A_j}, \quad (15)$$

$$A_i = \frac{a_i p}{R^2 T^2}, \quad (16)$$

$$B_i = \frac{b_i p}{RT}, \quad (17)$$

$$a_i = 0.45724 \frac{(RT_{c_i})^2}{p_{c_i}} \alpha, \quad (18)$$

$$b_i = 0.07780 \frac{RT_{c_i}}{p_{c_i}}, \quad (19)$$

$$\alpha = (1 + m * (1 - \sqrt{T_r}))^2, \quad (20)$$

$$T_r = \frac{T}{T_{c_i}}, \quad (21)$$

$$m = 0.03796 + 1.485 * w_i - 0.1644 * w_i^2 + 0.01667 * w_i^3 \quad (w_i > 0.4), \quad (22)$$

$$m = 0.37464 + 1.54226 * w_i - 0.26992 * w_i^2 \quad (w_i \leq 0.4), \quad (23)$$

where Z is the compressibility factor; p is the reservoir pressure; T is the reservoir temperature; R is the universal gas constant; T_r is the reduced temperature; T_{c_i} is the critical temperature of the component; p_{c_i} is critical component pressure; w_i is acentric factor; y_i is the mole concentration of the component in the mixture.

Thermal diffusion

The temperature gradient makes a significant contribution to the change in the composition of the hydrocarbon mixture. Taking into account the vertical temperature gradient leads, as a rule, to a stronger dependence of the initial composition on the depth than can be explained only by gravitational forces.

The effect of thermal diffusion on the distribution of the reservoir components is described using nonequilibrium thermodynamical models. Different approaches to considering the effect of thermal diffusion have been proposed by such authors as Belery and Da Silva (Belery, Da Silva, 1990), Haase (Haase, 1990), Kempers (Kempers, 1989), Whitson (Whitson, Belery, 1994), etc.

Pedersen and Lindeloff (Pedersen, Lindeloff, 2003) proposed the following relationships to calculate the compositional change with depth in reservoirs under the influence of gravity and thermal diffusion:

$$RT_2 \ln f_i(p, \vec{y})|_{h_2} = RT_1 \ln f_i(p, \vec{y})|_{h_1} + M_i g(h_1 - h_2) - M_i \left(\frac{H}{M} - \frac{\widetilde{H}_i}{M_i} \right) \frac{\Delta T}{T}, \quad i = 1, \dots, N, \quad (24)$$

where \widetilde{H}_i is the absolute partial molar enthalpy of i -th component, H is the absolute molar enthalpy of the mixture, M is the average molecular weight of the mixture, ΔT is the temperature difference between the depths h_2 and h_1 , T_1 is the temperature at the depth h_1 , T_2 is the temperature at the depth h_2 . Relation (24) corresponds to the nonequilibrium stationary state of the system in a gravitational and geothermal field.

The authors (Pedersen, Lindeloff, 2003) suggested that the change in component composition under stationary conditions and influence of the temperature gradient is determined by the specific enthalpy of each component. Components with a higher enthalpy than the average for the mixture tend to a warmer zone. Under typical reservoir conditions, high molecular weight components will have a higher specific enthalpy than low molecular weight ones. This corresponds to actual observations showing that the change in component composition with depth in reservoirs with a positive vertical temperature gradient is higher than can be explained only by the gravitational effect.

The partial molar enthalpy of i -th component in a mixture at temperature T can be represented by the following expression:

$$\widetilde{H}_i(T) = H_{i0}^{ig} + (H_i^{ig}(T) - H_{i0}^{ig}) + \widetilde{H}_i^{res}, \quad (25)$$

where $H_i^{ig}(T)$ и H_{i0}^{ig} is the partial molar enthalpy of i -th component in the ideal-gas state at temperatures T and 273.15 K, respectively, \widetilde{H}_i^{res} – is the partial residual molar enthalpy:

$$\widetilde{H}_i^{res} = -RT^2 \frac{\partial \ln \varphi_i}{\partial T}, \quad (26)$$

where φ is the fugacity coefficient of the i -th component.

Enthalpy of the i -th component in an ideal-gas state at a temperature of 273.15 K can be determined by the following formula:

$$\frac{H_i^{ig}(273.15K)}{R} = -134.2 + 8.367 * M_i, \quad (27)$$

and at temperature T , it can be determined from the following thermodynamic relation:

$$H_i^{ig}(T) - H_i^{ig}(273.15K) = \int_{273.15K}^T C_{P,i}^{id} dT, \quad (28)$$

where the heat capacity of an ideal gas is determined by the correlation with temperature:

$$C_{P,i}^{id} = C_{1,i}T + C_{2,i}T^2 + C_{3,i}T^3 + C_{4,i}T^4, \quad (29)$$

where the coefficients $C_{1,i}$ - $C_{4,i}$ are tabulated for C_1 - C_5 components of the mixture (Reid, Prausnitz, Poling, 1987). For C_{6+} components, the coefficients are calculated using Kesler-Lee empirical formulas (Kesler, Lee, 1976).

Vuktylskoye field

Based on the described model, calculation were performed for changes in the initial composition with depth for the main gas-condensate reservoir of the Vuktylskoye field with a large gas column (Tables 1-3). Fig. 1 shows the changes in the initial component composition of the gas-condensate mixture with the reservoir depth according to the data of (Dolgushin, 2007). The plots shown were obtained from actual data analysis of wells completed in the reservoir at various depths. Fig. 2 shows the change in the initial reservoir pressure and temperature over the depth of the reservoir. It is interesting to compare the dependences of the initial composition and pressure on the depth according to Fig. 1-2 and obtained by mathematical modeling. The latter are necessary as initial conditions for forecast simulations on a multicomponent 3D reservoir flow model.

	Constant temperature	Interval temperatures	Thermal diffusion
N ₂	5.45201	5.46618	6.09901
CO ₂	0.03593	0.03571	0.03625
C ₁	79.22680	79.31150	80.15020
C ₂	7.76406	7.72844	7.28671
C ₃	2.82648	2.80510	2.57673
iC ₄	0.33319	0.33012	0.30394
nC ₄	0.58375	0.57766	0.51958
iC ₅	0.10752	0.10618	0.09520
nC ₅	0.09297	0.09175	0.08075
C ₆₊₍₁₎	1.25377	1.23458	0.91920
C ₆₊₍₂₎	1.68256	1.68550	1.51376
C ₆₊₍₃₎	0.55714	0.54645	0.37851
C ₆₊₍₄₎	0.07829	0.07547	0.03763
C ₆₊₍₅₎	0.00534	0.00513	0.00244
C ₆₊₍₆₎	0.00021	0.00020	0.00011
P	33.04260	32.93150	33.02160

Table 1. Calculated component composition (molar fractions of the components in the mixture) at a depth of 2000 m

	Constant temperature	Interval temperatures	Thermal diffusion
N ₂	5.28145	5.28555	5.62076
CO ₂	0.03791	0.03784	0.03805
C ₁	77.43990	77.46610	78.24030
C ₂	8.13089	8.12082	7.86716
C ₃	3.11116	3.10486	2.95724
iC ₄	0.38162	0.38069	0.36201
nC ₄	0.67508	0.67320	0.63203
iC ₅	0.12954	0.12912	0.12066
nC ₅	0.11273	0.11233	0.10392
C ₆₊₍₁₎	1.58503	1.57859	1.33152
C ₆₊₍₂₎	2.09588	2.09788	1.94260
C ₆₊₍₃₎	0.84917	0.84494	0.67343
C ₆₊₍₄₎	0.15536	0.15387	0.10148
C ₆₊₍₅₎	0.01359	0.01345	0.00838
C ₆₊₍₆₎	0.00075	0.00074	0.00047
P	34.50070	34.47140	34.50690

Table 2. Calculated component composition (molar fractions of the components in the mixture) at a depth of 2500 m

	Constant temperature	Interval temperatures	Thermal diffusion
N ₂	4.68992	4.69193	4.18694
CO ₂	0.04139	0.04135	0.04100
C ₁	71.89110	71.90820	68.45650
C ₂	8.93229	8.92625	9.25570
C ₃	3.81971	3.81585	4.12125
iC ₄	0.50947	0.50890	0.56036
nC ₄	0.92533	0.92411	1.03742
iC ₅	0.19383	0.19354	0.22240
nC ₅	0.17162	0.17134	0.19968
C ₆₊₍₁₎	2.64608	2.64113	3.38334
C ₆₊₍₂₎	3.24845	3.25410	3.75229
C ₆₊₍₃₎	2.11299	2.10898	3.10978
C ₆₊₍₄₎	0.69862	0.69576	1.37629
C ₆₊₍₅₎	0.10599	0.10547	0.25513
C ₆₊₍₆₎	0.01317	0.01305	0.04189
P	37.34190	37.32690	37.38680

Table 3. Calculated component composition (molar fractions of the components in the mixture) at a depth of 3350 m

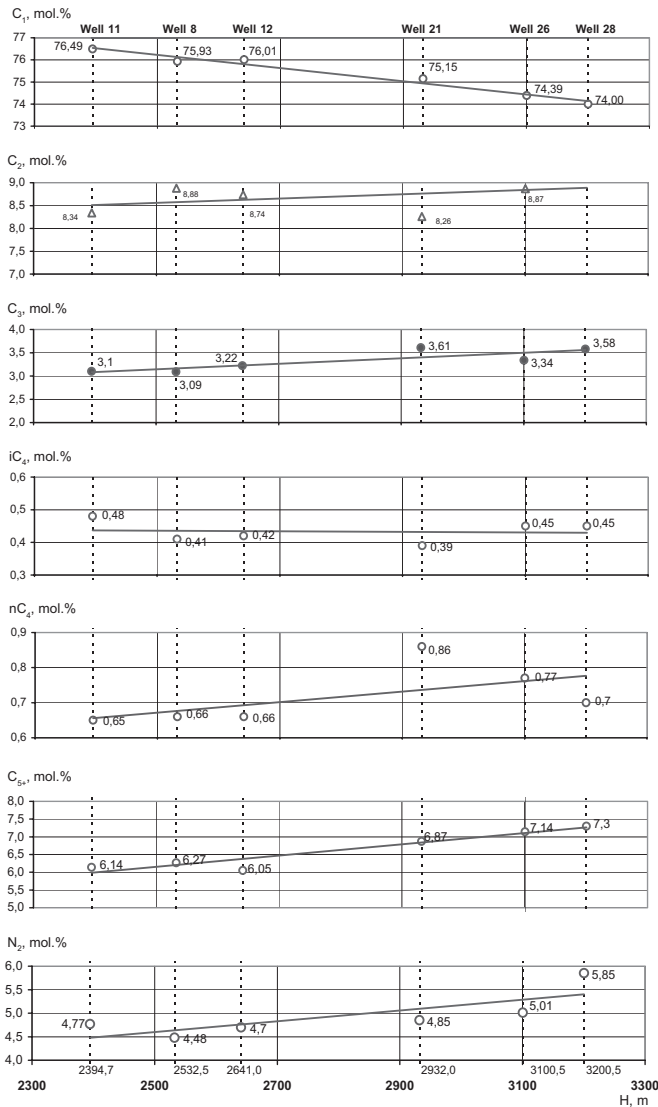


Fig. 1. Changes in the content of C₁, C₂, C₃, iC₄, nC₄, C₅₊, N₂ reservoir gas components within the vertical reservoir section for the initial conditions of the Vuktylskoye field (Dolgushin, 2007)

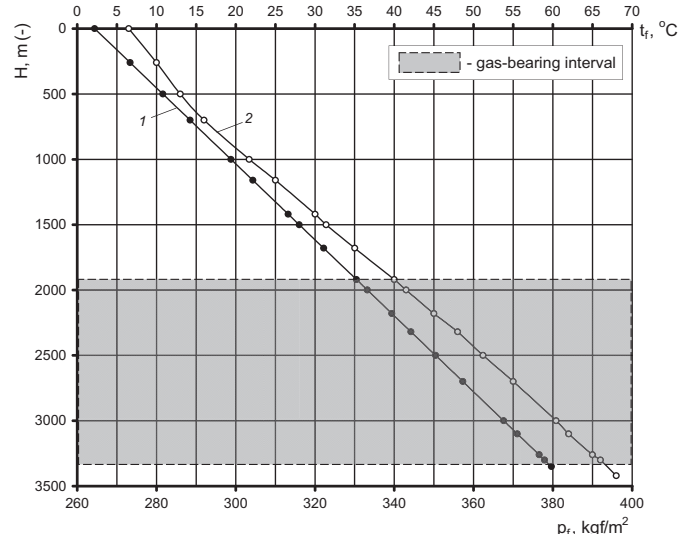


Fig. 2. Dependence of the initial values of reservoir pressure (1) and temperature (2) on the depth for the Vuktylskoye field (Dolgushin, 2007)

The model of the gas-condensate mixture was adopted according to the latest development design document (Supplement to the field development plan ..., 2014) and is represented by hydrocarbon components (methane, ethane, propane, butane, pentane and six fractions), as well as nitrogen and carbon dioxide (Table 4). At a depth of 3000 m, the initial composition of the mixture is known, the temperature of the reservoir is 334 K, the reservoir pressure is 36.1 MPa. Geothermal gradient equals to 0.019°C/m. Physical properties of hydrocarbon fractions are presented in Table 5. The goal is to recalculate the pressure and composition from the initial depth of 3000 m to a depth of 2000 m (upper level of the reservoir), 2500 m and 3350 m (gas-liquid contact).

Components	Mole fraction, %	Molar mass, kg/kmol	P, MPa	T, K	dT, °C/m
N ₂	5.01	28.01	36.1	334	0.019
CO ₂	0.04	44.01			
C ₁	74.85	16.04			
C ₂	8.56	30.07			
C ₃	3.47	44.1			
iC ₄	0.45	58.12			
nC ₄	0.8	58.12			
iC ₅	0.16	72.15			
nC ₅	0.14	72.15			
C ₆₊₍₁₎	2.08	85.02			
C ₆₊₍₂₎	2.67	110.46			
C ₆₊₍₃₎	1.38	157.95			
C ₆₊₍₄₎	0.35	231.22			
C ₆₊₍₅₎	0.0404	338.18			
C ₆₊₍₆₎	0.0034	500			

Table 4. Model of gas condensate mixture and input data at a depth of 3000 m (Supplement to the field development plan ..., 2014)

Fraction	Density, g/cm ³	Critical temperat., Tc, K	Critical pressure Pc, MPa	Acentric factor ω	Molar concentration of the component in the mixture z	M, g/mol	Boiling temperature, Tb, K
C6+(1)	0.664	504.9	3.060	0.2923	0.02082	85.0188	339.126
C6+(2)	0.708	570.4	2.505	-0.2581	0.02668	110.457	399.174
C6+(3)	0.750	646.6	1.941	0.3433	0.01381	157.954	474.645
C6+(4)	0.787	732.4	1.382	0.8143	0.003451	231.218	569.612
C6+(5)	0.821	818.6	0.946	1.0015	$4.04 \cdot 10^{-4}$	338.184	673.787
C6+(6)	0.854	904.8	0.645	1.2589	$3.36 \cdot 10^{-5}$	500	783.105

Table 5. Physical properties of fractions (Supplement to the field development plan ..., 2014)

The calculations were carried out using the following three methods:

- 1) Gravity method – the equation (1),
- 2) Taking into account the interval temperature change, but without thermal diffusion,
- 3) Taking into account thermal diffusion – the equation (24).

Calculation results

Fig. 3-10 show some calculation results. The depth changes of pressure and initial concentrations of gas-condensate mixture individual components are given for the main reservoir of the Vuktylskoye field. Fig. 9 corresponds to the group of C₅₊ hydrocarbons, i.e. the sum of pentanes and all C₆₊ fractions.

The concentration of light components (nitrogen and methane) decreases with depth (Fig. 3-4), while the concentration of heavier hydrocarbons starting with ethane increases with depth (Fig. 5-9). The higher the molecular weight of the component, the more its content increases with depth. Initial reservoir pressure changes consistently (Fig. 10). These features are associated with the influence of the gravitational field and are predominant in all variants of calculations.

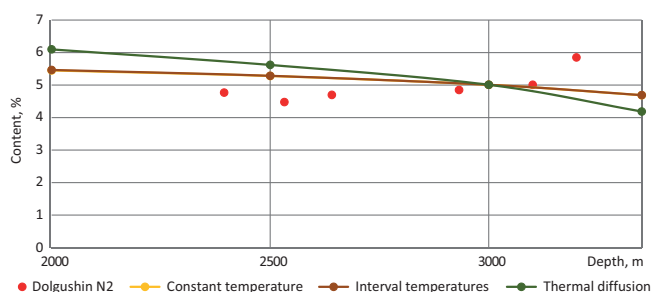


Fig. 3. Change in nitrogen content with depth

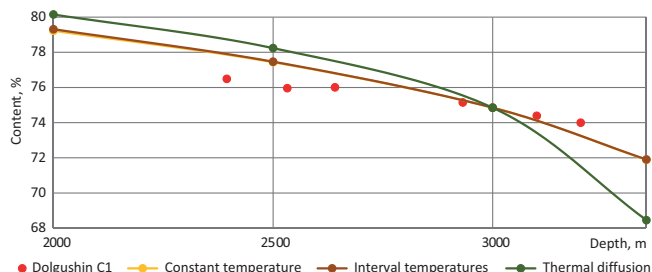


Fig. 4. Change in methane content with depth

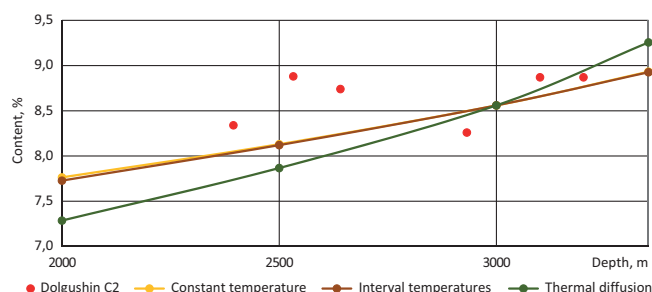


Fig. 5. Change in ethane content with depth

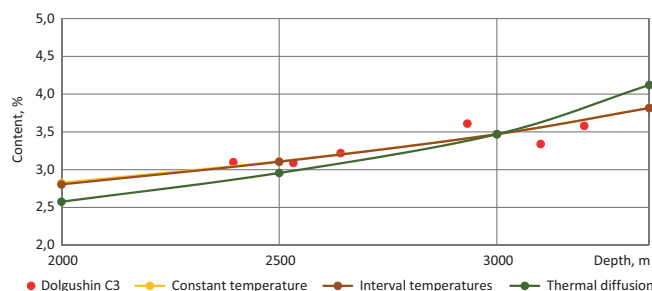


Fig. 6. Change in propane content with depth

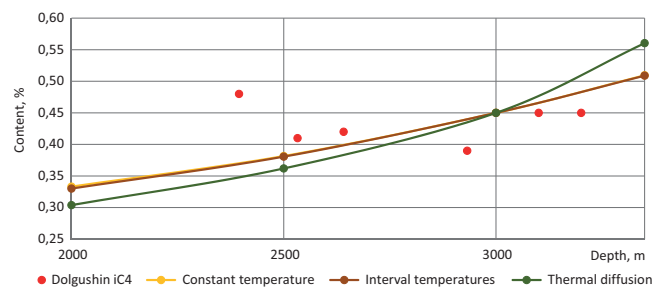


Fig. 7. Change in iso-butane content with depth

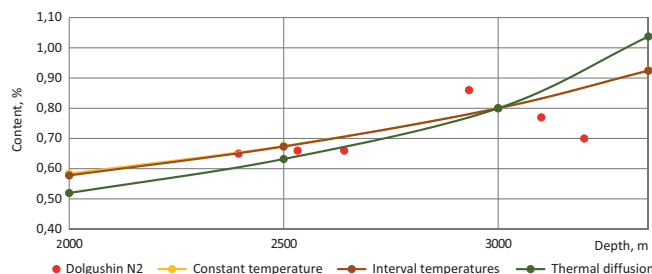


Fig. 8. Change in normal-butane content with depth

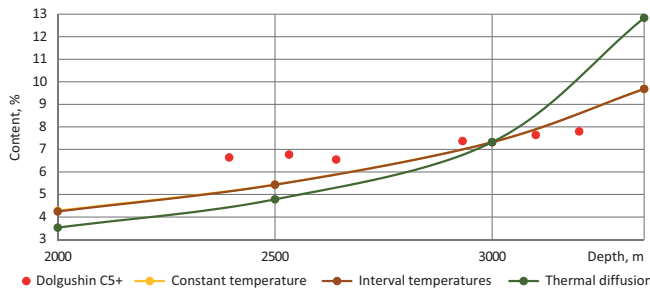


Fig. 9. Change in content of group of components C_{5+} with depth

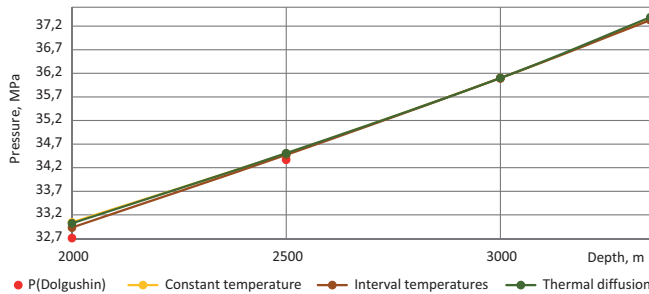


Fig. 10. Change in initial reservoir pressure with depth

From Fig. 3-10, it can be seen that when taking into account the temperature variation, the obtained composition distribution with depth is only slightly different from the isothermal case. This result confirms the conclusions of the work (Whitson, Belery, 1994).

Also from Fig. 3-10, it follows that the effect of thermal diffusion is essential and enhances the gravitational field influence for the described hydrocarbon system. A similar result was obtained in (Pedersen, Hjerstad, 2006) for another reservoir, where it was shown to match the actual data. The same method to account for thermal diffusion was used. However, this conclusion should not be absolutized, since a number of other authors indicate that thermal diffusion can reduce the influence of the gravitational field. In any case, it is characteristic that the composition changes with depth taking into account thermal diffusion become essentially nonlinear.

From Fig. 3-6, it can be seen that the data calculated by the gravitational method of the composition distribution and the interval-wise temperature consideration do not agree well with the actual data presented by N.V. Dolgushin (Dolgushin, 2007). Accounting for the effect of thermal diffusion also does not give a satisfactory approximation, and for a number of components it makes bigger the observed deviation.

Thus, the physical mechanisms causing the initial distribution of the component composition with depth for the Vuktylskoye field require further analysis. In particular, it is advisable to take into account the possible effect of the residual liquid hydrocarbon phase, the effect of the adopted component model

of the mixture and to try other models for describing thermal diffusion.

On the other hand, it should be taken into account that information on the distribution of the composition according to well data (Dolgushin, 2007) is also not the result of direct measurements. It is obtained by analyzing and averaging the well performance data with significant (hundreds of meters) production intervals in a heterogeneous reservoir. It is also important that N.V. Dolgushin made some assumptions regarding the possibility of relying on data on the well production composition at certain dates as an estimate of the initial distribution.

Conclusions

The paper considers mathematical modeling of changes in the initial component composition of hydrocarbon mixtures with depth in massive reservoirs under the influence of natural physical fields (gravitational and geothermal).

Numerical algorithms have been implemented to calculate the distribution of hydrocarbon mixture components over depth in the gravitational field under isothermal conditions, or taking into account interval temperature variation and thermal diffusion.

The results of comparative calculations for the main gas-condensate reservoir mixture of the Vuktylskoye field showed that thermal diffusion has a significant effect on the distribution of components, as well as the initial reservoir pressure. In the case under consideration, thermal diffusion magnifies the influence of the gravitational field and leads to pronounced non-linear dependencies for the components concentrations.

Satisfactory agreement of the calculations results with the component composition distribution according to well operation data was not achieved for any of the algorithms. The physical mechanisms determining the distribution of the initial composition within the reservoir volume of the Vuktylskoye field require further analysis.

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About the Authors

Anton V. Yashin – Engineer, MSc student
Gubkin Russian State University of Oil and Gas
(National Research University)

Oil and Gas Research Institute of the Russian Academy
of Sciences

3, Gubkin st., Moscow, 119333, Russian Federation

Ilya M. Indrupskiy – DSc (Engineering), Professor,
Head of Laboratory

Gubkin Russian State University of Oil and Gas
(National Research University)

Oil and Gas Research Institute of the Russian Academy
of Sciences

3, Gubkin st., Moscow, 119333, Russian Federation

Olga A. Lobanova – PhD (Engineering), Researcher
Oil and Gas Research Institute of the Russian Academy
of Sciences

3, Gubkin st., Moscow, 119333, Russian Federation

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