Mathematical modeling of gas-condensate mixture filtration in porous media taking into account non-equilibrium of phase transitions

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Abstract. At the present time, a considerable part of the largest dry gas reservoirs in Russia are found in the stage of declining production, therefore active exploitation of gas-condensate fields will begin in the coming decades. There is a significant discrepancy between the project and the actual value of condensate recovery factor while producing reservoir of this type, which is caused by insufficient knowledge about non-equilibrium filtration mechanisms of gas-condensate mixtures in reservoir conditions. A system of differential equations to describe filtration process of two-phase multicomponent mixture for one-, two- and three-dimensional cases is presented in this work. The solution of the described system was made by finite-element method in the software package FlexPDE. Comparative distributions of velocities, pressures, saturations and phase compositions of three-component mixture along the reservoir model and in time in both cases of equilibrium and non-equilibrium filtration processes were obtained. Calculation results have shown that system deviation from the thermodynamic equilibrium increases gas phase flow rate and reduces liquid phase flow rate during filtration process of gas-condensate mixture.

1. Introduction
In order to enhance existing and implement new hydrocarbon production methods and to enhance the efficiency of the field development process control, there is an increased need in conducting in-depth theoretical and experimental studies of the specifics of non-equilibrium filtration of reservoir fluids in porous medium [1–3]. These fluids are multicomponent multiphase mixtures of hydrocarbon and non-hydrocarbon components (nitrogen, hydrogen sulfide, water). In-depth investigation and understanding of the filtration flows of such mixtures accompanied by a number of complex physical and chemical phenomena taking place during various processes of oil, oil-gas, and oil-gas-condensate reservoirs development are required in order to determine the methods of implementation of such processes and specific recommendations concerning the control of development processes [4–6].

In this context, correct and physically and chemically justified statement of the mathematical model of multicomponent hydrocarbon mixture filtration with regard to diffusion flows in phases and non-equilibrium kinetics of interphase mass transfer processes allows not only to track instability of gas-condensate field operation, but also to provide recommendations concerning the control of actual multicomponent field development process at the macro level [2,3,7].

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A mathematical model of the process of non-equilibrium filtration of a 2-phase \( N \)-component hydrocarbon mixture in a porous medium, taking into account inertia forces, phase transitions, capillary and diffusion effects is described in detail in works [8, 9]. The aim of this study was to establish and to refine the system of initial differential equations taking into account the effects influencing on non-equilibrium. This article presents a system of differential equations for a 2-phase isothermal filtration of \( N \)-component mixture for one-, two-, and three-dimensional cases, the solution of which allows determining pressures and mass fractions of components in phases.

2. Mathematical model

2.1. Phase flow equation and mass conservation law of mixture component

Let us write motion equations of a continuous medium element with regard to inertia forces [10–12] and mass conservation equations of the \( i \)-th component in the G-phase (gas phase) and C-phase (liquid phase):

\[
\rho_g \frac{\partial}{\partial t} u_g + \frac{\mu_g m}{k} u_g = -\nabla P_g; \tag{1}
\]

\[
\rho_c \frac{\partial}{\partial t} u_c + \frac{\mu_c m}{k} u_c = -\nabla P_c; \tag{2}
\]

\[
\text{div} (u_g \rho_g G_i + Q^g_i) - V_i + \frac{\partial}{\partial t} (m S_g \rho_g G_i) = 0; \tag{3}
\]

\[
\text{div} (u_c \rho_c C_i + Q^c_i) + V_i + \frac{\partial}{\partial t} (m S_c \rho_c C_i) = 0; \tag{4}
\]

where \( i = 1, \ldots, N; \rho_g, \rho_c \) —densities of G-phase and C-phase; \( \mu_g, \mu_c \) —viscosities of G-phase and C-phase; \( P_g, P_c \) —pressures of G-phase and C-phase; \( u_g, u_c \) —velocities of G-phase and C-phase; \( m \) —reservoir porosity; \( k \) —reservoir permeability; \( \nabla \) —nabla operator; \( G_i, C_i \) —mass fraction of \( i \)-th component of G-phase and C-phase; \( Q^g_i, Q^c_i \) —diffusion fluxes of \( i \)-th component in G-phase and C-phase; \( V_i \) —transfer rate of \( i \)-th component from one phase to another; \( S_g, S_c \) —saturations of the porous medium with G-phase and C-phase.

Taking the gradient of chemical potential as the moving force of the isothermal molecular diffusion, we obtain for the diffusion flow of the \( i \)-th component in the G-phase and C-phase [13]:

\[
Q^g_i = -D^g_i \nabla \phi^g_i; \tag{5}
\]

\[
Q^c_i = -D^c_i \nabla \phi^c_i, \tag{6}
\]

where \( i = 1, \ldots, N; D^g_i, D^c_i \) —diffusion coefficients for \( i \)-th component in G-phase and C-phase; \( \phi^g_i, \phi^c_i \) —Gibbs energy for \( i \)-th component in G-phase and C-phase.

The transfer rate of the \( i \)-th component through the interphase surface from the phase with the higher chemical potential to the phase with the lower chemical potential for the same component is determined by the difference of potentials and expressed by equation [14, 15]:

\[
V_i = \eta_i (\phi^c_i - \phi^g_i), \tag{7}
\]

where \( \eta_i \) —interphase transfer coefficient.

Note that the viscosities and densities of phases in equations (1)–(4), as well as chemical potentials, substance diffusion and phase transfer coefficients included in equations (5)–(7), are determined experimentally and depend on the mixture composition, phase saturation, pressure,
and temperature:

\[ \mu_g = \mu_g(G_1, G_2, \ldots, G_N, P_g); \]  
\[ \mu_c = \mu_c(C_1, C_2, \ldots, C_N, P_c); \]  
\[ \rho_g = \rho_g(G_1, G_2, \ldots, G_N, P_g); \]  
\[ \rho_c = \rho_c(C_1, C_2, \ldots, C_N, P_c); \]  
\[ D_g^i = D_g^i(G_1, G_2, \ldots, G_N, P_g, S_g); \]  
\[ D_c^i = D_c^i(C_1, C_2, \ldots, C_N, P_c, S_c); \]  
\[ \phi_g^i = \phi_g^i(G_1, G_2, \ldots, G_N, P_g, T); \]  
\[ \phi_c^i = \phi_c^i(C_1, C_2, \ldots, C_N, P_c, T). \]  

By virtue of the identities expressing the balance of mass fractions and saturations in the G-phase and C-phase:

\[ \sum_{i=1}^{N} G_i = 1; \]  
\[ \sum_{i=1}^{N} C_i = 1; \]  
\[ S_g + S_c = 1. \]  

Only the mass fractions of \((N - 1)\) components and the saturation of one phase are independent of one another.

The difference of pressures \(P_g, P_c\) in the G-phase and C-phase is the capillary pressure at the boundary between the G- and C-phases:

\[ P_c - P_g = P_{\text{capillary}}. \]  

Note that the system of equations (1)–(4) is transformed into a system corresponding to equilibrium phase transitions with \(\phi_i^g = \phi_i^g(\eta_i \to \infty)\) and ignorance of diffusion terms.

### 2.2. System of one-dimensional equations and phase transfer coefficient

Let us write the system of 2-phase mixture filtration equations (1), (2) and N-component mass conservation equations (3), (4) for the one-dimensional case (using the Ox axis) with regard to non-equilibrium kinetics of phase mass transfer and diffusion exchange in phases:

\[ \rho_g \frac{\partial}{\partial t} u_g + \mu_g \frac{m_k}{k} u_g = -\frac{\partial}{\partial x} P_g; \]  
\[ \rho_c \frac{\partial}{\partial t} u_c + \mu_c \frac{m_k}{k} u_c = -\frac{\partial}{\partial x} P_c; \]  
\[ \frac{\partial}{\partial x} (u_g \rho_g G_i + Q_i^g) - V_i + \frac{\partial}{\partial t} (mS_g \rho_g G_i) = 0; \]  
\[ \frac{\partial}{\partial x} (u_c \rho_c C_i + Q_i^c) + V_i + \frac{\partial}{\partial t} (mS_c \rho_c C_i) = 0; \]

\(i = 1, \ldots, N.\)

The system (20)–(23) with regard to capillary pressure equation (19) and composition and saturation balance equations (16)–(18) is a closed system of \(2N + 2\) equations in the following unknowns: phase velocities \(u_g, u_c\), pressure \(P_g\) (or \(P_c\)), gas saturation \(S_g\) (or \(S_c\)), the mass
fractions of components in phases $G_1, G_2, \ldots, G_{n-1}, C_1, C_2, \ldots, C_{n-1}$. To enable calculations using equations (20)–(23), besides the equilibrium phase relations and the physical properties of phases, substance phase transfer coefficients $\eta_i$ must also be known. For actual oil-gas and gas-condensate fields, the substance phase transfer coefficients $\eta_i$, describing the existence of non-equilibrium processes in the mixture depend on the characteristic of the porous medium, as well as pressure, saturation, and phase composition. Determining these coefficients requires special complex laboratory experiments in multicomponent mixture filtration, involving the measurement of the distributions of pressures, component concentrations in phases, and saturation [9]. Diffusion coefficients are determined using existing experimental data available in literature. If such data are not available, these coefficients are determined by calculation [16].

3. Numerical computation using FlexPDE software package

Let us consider the process of 3-component methane–propane–heptane mixture filtration through a porous medium. A 0.3 m long core is pre-filled with liquid heptane $C_7H_{16}$, which is in the equilibrium condition. After that a binary methane–propane mixture ($CH_4–C_3H_8$) is injected into the core at a pressure of 10 MPa. Constant quantities of the two non-equilibrium phases with given constant compositions are specified for the core inlet: $G_m = 0.9$, $G_p = 0.1$ (from this point onward, the “m” subscript is used for methane, the “p” subscript—for propane, and the “h” subscript—for heptane).

From (20)–(23) we obtain the following system of 8 equations for 3-component mixture:

\[
\begin{align*}
\rho_g \frac{\partial}{\partial t} u_g + \frac{\mu_m}{k} u_g G_m &- \frac{\partial}{\partial x} P_g = 0; \\
\rho_c \frac{\partial}{\partial t} u_c + \frac{\mu_m}{k} u_c C_m &- \frac{\partial}{\partial x} P_c = 0; \\
\frac{\partial}{\partial x} (u_g \rho_g G_m + Q_m) - V_m + \frac{\partial}{\partial t} (mS_g \rho_g G_m) &= 0; \\
\frac{\partial}{\partial x} (u_g \rho_g G_p + Q_p) - V_p + \frac{\partial}{\partial t} (mS_g \rho_g G_p) &= 0; \\
\frac{\partial}{\partial x} (u_g \rho_g G_h + Q_h) - V_h + \frac{\partial}{\partial t} (mS_g \rho_g G_h) &= 0; \\
\frac{\partial}{\partial x} (u_c \rho_c C_m + Q_m) + V_m + \frac{\partial}{\partial t} (mS_c \rho_c C_m) &= 0; \\
\frac{\partial}{\partial x} (u_c \rho_c C_p + Q_p) + V_p + \frac{\partial}{\partial t} (mS_c \rho_c C_p) &= 0; \\
\frac{\partial}{\partial x} (u_c \rho_c C_h + Q_h) + V_h + \frac{\partial}{\partial t} (mS_c \rho_c C_h) &= 0.
\end{align*}
\]

The system of one-dimensional equations (25)–(32) for 2-phase 3-component mixture methane–
propane–heptane, with regard to capillary pressure equation (19) and composition and saturation balance equations (16)–(18) is a closed system of 12 equations in the following unknowns: phase velocities \( u_g \), \( u_c \), pressure \( P_g \) (or \( P_c \)), gas saturation \( S_g \) (or \( S_c \)) and four of the six mass fractions of components in phases. Parameters (8)–(15), included in equations (25)–(32), were determined experimentally.

4. Results of numerical computation

The described equation system was solved utilizing the finite element method using the FlexPDE software package. Comparative distributions of pressures and the composition of 3-component mixture phase in time were obtained, both for the equilibrium filtration process and taking non-equilibrium into consideration. The system of equations (25)–(32) was solved by splitting the domain into 60 cells (figure 1). 16 computation cycles with a current time step (Dt) – 7.07 s were required. The current estimated RMS error was \( 9.81 \times 10^{-6} \), the current estimated max error was \( 1.34 \times 10^{-5} \).

The comparison of the pressure and flow rate curves with regard to thermodynamic non-equilibrium and with chemical potentials of phases being equal demonstrates qualitative
differences of the distribution of both pressure and flow rates (figures 2–5; blue lines are for equilibrium flow, red lines are for non-equilibrium one).

Computation results demonstrate that the pressure and flow rates of the liquid phase components of the mixture at the outlet cross-section ($x = 0.3$ m) by the 60-th minute of the process of mixture injection into the core have different values with equilibrium and non-equilibrium filtration processes; it was observed that system deviation from the thermodynamic equilibrium led to increased gaseous phase flow rate and decreased liquid phase flow rate during gas-condensate mixture filtration.

5. Conclusions
A one-dimensional mathematical model of the isothermal filtration process of two-phase three-component mixture methane–propane–heptane was developed based on the mathematical model of the non-equilibrium filtration process of two-phase $N$-component hydrocarbon mixture in a porous medium. The model developed was implemented in the FlexPDE software package. Numerical computation results demonstrate qualitative differences of the distribution of both pressure and flow rates of the liquid phase components, both with and without regard to process non-equilibrium. To enable obtaining more accurate quantitative results, experimental studies of multicomponent mixture filtration are required in order to determine diffusion and substance phase transfer coefficients.

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