One-dimensional continuum model of two-phase flows in porous media

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Abstract. We present analytical and numerical description of two-phase flows in a porous medium for one-dimensional case. This research is aimed at modeling of natural gas condensate flows at hydrocarbon reservoir conditions. The model is component-scalable, uses generalized cubic equation of state and assumes equal pressures in coexisting phases. It can be used for miscible and immiscible fluid in a unified way. First results for binary mixture flows of alkanes are provided including self-oscillatory regime.

1. Introduction
Multiphase filtration processes in porous media occur during the exploitation of hydrocarbon deposits. One of the complex cases of numerical simulation is a retrograde condensation flow. The non-linear behavior of the gas solubility in liquid plays a major role in that case. Development of new numerical approaches has a value of its own, but the goal of both numerical and experimental studies is debit increase.

Experimental studies reported two regimes of filtration of gas-condensate binary mixture [1]. Both regimes have flow rate oscillations and correspond to the retrograde region of the mixture. In the first regime, pressure drop within the experimental section is high and the oscillations stop. In the second regime, the pressure drop is smaller and the oscillations continue. Those experiments hint at the possibility of self-oscillatory flow modes in the system.

The current paper describes a numerical model of a two-phase flow in a porous media. The model extends the binary mixture flow model proposed in [2]. We formulate hydrodynamic equations with respect to densities of components in two-phase state. Moreover, we assume local thermodynamical equilibrium. Consequently, we dispense with calculation of mass exchange between the phases. Our model noticeably differs from [2] in two features. Firstly, we consider the volume constraint in determining the equilibrium. Secondly, we require the densities of the substances to be consistent with pressure at the right boundary.

We present numerical tests for a binary mixture with the generalized cubic equation of state (EoS) [3]. The EoS accurately describes fluids at hydrocarbon reservoir conditions.
2. Miscible fluids

2.1. Continuity equation in porous media

We derive the equations for the two-phase one-dimensional (1D) flow of a multicomponent fluid. The amount of a substance \( \nu_c \) in a homogenous fluid could be expressed as a space integral of molar concentration \( n_c \) over volume of the fluid \( V_c \):

\[
\nu_c = \int_{V_c} n_c \, dw.
\]  

(1)

Let us consider a multi-component fluid separated into the gas (g) and liquid (l) phases and located in a porous media with constant porosity \( m \). In this case, the amount \( \nu_c \) of a component \( c \) is the sum of its amounts in both phases:

\[
\nu_c = m \int_V \left[ \alpha_{g,c} n_g s + \alpha_{l,c} n_l (1 - s) \right] \, dw,
\]  

(2)

where \( V \) is the volume of the porous media including pores, \( \alpha_{ph,c} \) is the molar fraction of component \( c \) in phase \( ph \), \( \sum_c \alpha_{ph,c} = 1 \), \( ph = \{g, l\} \), \( n_{ph} \) is molar concentration of phase \( ph \), and \( s \) is the gas saturation (volume of gas divided by volume of pores).

We denote by \( Y_c \) the quantity under the integral (2):

\[
Y_c = \alpha_{g,c} n_g s + \alpha_{l,c} n_l (1 - s).
\]  

(3)

The continuity equation for the component \( c \) in the 1D case can be written as follows:

\[
m \partial_t Y_c + \partial_x j_c = 0,
\]  

(4)

\[
\partial_x j_c = \alpha_{g,c} n_g u_g + \alpha_{l,c} n_l u_l,
\]  

(5)

where \( t \) is time variable, \( x \) is space variable and \( u_{ph} \) is filtration velocity of the fluid phase \( ph \).

We approximate the filtration velocities of the phases \( u_{ph} \) by the Darcy’s law:

\[
u_{ph} = -\frac{k f_{ph}(s)}{\eta_{ph}} \frac{\partial P}{\partial x},
\]  

(6)

where \( k \) is absolute permeability, \( f_{ph} \) and \( \eta_{ph} \) are the relative permeability function and the dynamic viscosity of \( ph \) phase.

The equations are completed by the EoS:

\[
P V_{ph} = z_{ph}(P, T, \alpha_{ph,c}) \nu_{ph} RT,
\]  

(7)

where \( V_{ph}, z_{ph}, T, \nu_{ph} \) are volume, super-compressibility, temperature and amount of phase \( ph \) respectively, \( R \) is the ideal gas constant. We denote the chemical potential of component \( c \) in phase \( ph \) by \( \varphi_{ph,c}(P, T, \alpha_{ph,c}) \). It can be derived analytically from the EoS.

Below, we clarify the description of the two-component fluid. The temperature profile \( T = T(x,t) \) is assumed to be given. The two-component isothermal case follows experimental conditions in [1]. However, the model is component-scalable in clear way. The pressures of both phases are considered equal.

Computation of the phase equilibrium, given the amounts \( Y_1, Y_2 \) of the components per unit volume at a given temperature \( T \), is equivalent to the system for pressure \( P \) and molar fractions \( \alpha_{ph,c} \):

\[
\varphi_{g,c}(P, T, \alpha_{g,c}) = \varphi_{l,c}(P, T, \alpha_{l,c}),
\]  

(8)

\[
\frac{P}{RT} = (Y_1 + Y_2)[z_g(P, T, \alpha_{g,c})G(P,T, \chi) + z_l(P,T,\alpha_{l,c})(1 - G(P,T, \chi))],
\]  

(9)

where \( \chi \) is the molar fraction of component 1 in mixture, \( G \) and \( 1 - G \) are molar fractions of gas and liquid phases in the mixture, respectively. The molar fraction \( \chi \) could be found directly from \( Y_1, Y_2 \):

\[
\chi \overset{\text{def}}{=} \frac{\nu_1}{\nu_1 + \nu_2} = \frac{Y_1}{Y_1 + Y_2}.
\]  

(10)
The volume fraction of gas $s$ relates to its molar fraction $G$ as follows

$$s = \frac{z_g G}{z_g G + z_i (1 - G)}.$$  \hspace{1cm} (11)

The initial and boundary conditions imitate the experimental statement of the filtration problem:

$$P(x, 0) = P_{in}, \quad \chi(x, 0) = \chi_{in},$$  \hspace{1cm} (12)

$$P(0, t) = P_{in}, \quad \chi(0, t) = \chi_{in},$$  \hspace{1cm} (13)

$$P(L, t) = \begin{cases} P_{in} + (t/t_r)(P_{out} - P_{in}) & \text{for } 0 \leq t < t_r, \\ P_{out} & \text{for } t \geq t_r. \end{cases}$$  \hspace{1cm} (14)

The boundary condition for pressure at the right boundary (14) needs additional attention. Firstly, we use time relaxation to avoid discontinuities at initial stage. Secondly, unlike the region $x = (0, L)$ the pressure $P(L, t)$ is known, so the quantities of components $Y_c(L, t)$ have to satisfy the phase equilibrium conditions (8) and (9).

2.2. Numerical model

Let us define space and time grids:

$$\omega_h = \{x_i \in \mathbb{R} : x_i = (i - 1)h, h > 0, h(N - 1) = L, i = 1, 2, \ldots, N\},$$  \hspace{1cm} (15)

$$\omega_r = \{t_j \in \mathbb{R} : t_j = j\tau, \tau > 0, j = 0, 1, \ldots\}.$$  \hspace{1cm} (16)

The equations (4), (5), (6) are approximated by the following explicit finite-difference scheme:

$$m \frac{\hat{Y}_{c,i} - Y_{c,i}}{\tau} = \frac{1}{h} \left[ a_{c,i+1/2} \frac{P_{i+1} - P_i}{h} - a_{c,i-1/2} \frac{P_i - P_{i-1}}{h} \right],$$  \hspace{1cm} (17)

$$a_{c,i+1/2} = 0.5(a_{c,i} + a_{c,i-1}),$$  \hspace{1cm} (18)

$$a_{c,i} = \frac{k_f(s_i)}{\eta_{g,i}} + \alpha_i l_i n_{\eta,i},$$  \hspace{1cm} (19)

where $i = 2, \ldots, N - 1$.

Here, the independent variables are $Y_1$ and $Y_2$, pressures and gas saturations are calculated from them using the equation of state.

The left boundary condition $\hat{Y}_{c,0}$ is determined from known phase equilibrium at $x = 0$ (13) and the definition of $Y_c$ (3).

On the right boundary, we synthetically reduce the amount of substances $Y_1(L, t) + Y_2(L, t)$ to satisfy the right boundary pressure $P(L, t)$. This procedure imitates a pressure regulator idea. Hence, the right boundary $\hat{Y}_{c,N}$ is calculated as follows

$$\hat{Y}_{c,N} = Y_{c,N} - 2\tau/(hm)a_{c,N-1/2}(P_N - P_{N-1})/h,$$  \hspace{1cm} (20)

$$\chi_N = \hat{Y}_{1,N}/(\hat{Y}_{1,N} + \hat{Y}_{2,N}),$$  \hspace{1cm} (21)

$$\hat{Y}_{1,N} = \hat{\chi}_N(P_N/RT)/\left(\hat{z}_{g,N}\hat{G}_N + \hat{z}_{i,N}(1 - \hat{G}_N)\right),$$  \hspace{1cm} (22)

$$\hat{Y}_{2,N} = \hat{Y}_{1,N}/\hat{\chi}_N(1 - \hat{\chi}_N).$$  \hspace{1cm} (23)

Here we count the flux at $N - 1/2$, which enters $N$ grid point. Then we approximate the estimated molar part of component 1 $\hat{\chi}_N$ in order to determine phase equilibrium at $N$ from $P_N, \hat{\chi}_N$, and $T$. After that, we find $\hat{Y}_{c,N}$ which satisfies (8) and (9). The value $0.5h(\hat{Y}_{c,N} - \hat{Y}_{c,N})/\tau > 0$ is treated as the flow rate at the edge $x = L$.

To solve (8) and (9), we use the phase equilibrium algorithm described in [3]. In the case of binary mixture, it can be expressed in form of a function:

$$(P, T, \chi, \text{components info}) \rightarrow (z_g, z_i, \hat{V}, \hat{L}, \alpha_{g,1}, \alpha_{i,1}, \alpha_{g,2}, \alpha_{i,2}).$$  \hspace{1cm} (24)
Here “components info” is set of parameters which determine the EoS of pure components. It includes critical pressure $P_{cr}$, critical temperature $T_{cr}$, and the fitting parameters $Z_{cr}^*$, $\Omega_{cr}$, $\psi$.

After finding $\hat{Y}_c = Y_c(x, t + \tau)$ in $\omega_h$, the fluxes in (17) could be found via the following procedure:

- Find $\hat{\chi}$ from (10).
- Find $\hat{P}$ that satisfies (9) for $\hat{Y}_c$ and $\hat{\chi}$ using (24). After that, $\hat{z}_{ph}, \hat{G}, \hat{\alpha}_{ph,c}$ for $c = \{1, 2\}$ and $ph = \{g, l\}$ are known too.
- Calculate molar concentrations as follows from (7)
  $$\hat{n}_{ph} = \frac{\hat{P}}{\hat{z}_{ph} RT}.$$  
(25)
- Find $\hat{s}$ (11),
  $$\hat{s} = \frac{\hat{z}_g \hat{G}}{\hat{z}_g \hat{G} + \hat{z}_l (1 - \hat{G})},$$  
(26)
and calculate the next coefficients $\hat{a}_{c,i}$ (19).

3. Immiscible 2-component fluid

In the simplest case, the gas phase consists of pure component 1 and the liquid phase of pure component 2, so the equations simplify:

$$\alpha_{l,1} = \alpha_{l,2} = 1, \quad \alpha_{l,1} = \alpha_{g,2} = 0,$$
(27)
$$G = \chi,$$
(28)
$$Y_1 = n_1 s, \quad Y_2 = n_2 (1 - s).$$
(29)

Since $n_c = v_c^{-1}$ for $c = \{1, 2\}$ and (29), the procedure of finding pressure from (9) may be replaced. It is more natural to calculate pressures directly from cubic form of $P(v, T)$ [3]:

$$P_c(v_c, T) = \frac{RT}{v_c - b_c} - \frac{\tilde{a}_c(T)}{(v_c + c_c)(v_c + d_c)}, \quad c = \{1, 2\},$$
(30)

where $\tilde{a}_c(T), b_c, c_c, d_c$ are EoS coefficients of the components.

Hence, $\hat{P}$ and $\hat{s}$ can be found from

$$P_1(v_1(s)) - P_2(v_2(s)) = 0,$$
(31)
$$v_1(s) = \frac{s}{Y_1}, \quad v_2(s) = \frac{1 - s}{Y_2},$$
(32)
where the root of (31) is localized in area $\{s : v_1(s) > b_1, v_2(s) > b_2\}$. We use Ridders’ root-finding solver [4] for that system. Finally, the value of $\hat{n}_c$ could be determined via (29) with $\hat{Y}_c$ and $\hat{s}$.

4. Results and discussion

4.1. Immiscible 2-component fluid

We implemented the numerical model described in section 3.

A numerical test for a mixture of nitrogen $N_2$ and n-octane $n-C_8H_{18}$ was conducted. The parameters of the test and the mixture are provided in tables 1 and 2. In this test, we used constant viscosities.

The molar composition and pressure drop allow both phases to flow through the medium at all values of space $x$ and time $t$. The steady state is rapidly achieved at $t \approx 20$ s. The gas
Table 1. EoS parametrization of pure components.

| Substance | $P_{cr}$ (bar) | $T_{cr}$ (K) | $Z_{cr}^*$ | $\Omega_{cr}$ | $\psi$ |
|-----------|----------------|--------------|----------|--------------|------|
| nitrogen  | 33.9           | 126          | 0.34626  | 0.75001      | 0.37182 |
| n-octane  | 24.9           | 569          | 0.32412  | 0.75001      | 1.16619 |
| methane   | 46             | 191          | 0.33294  | 0.75630      | 0.37447 |
| n-butane  | 38             | 425          | 0.31232  | 0.76921      | 0.57594 |

Table 2. Parameters of the numerical tests for immiscible (I) and miscible (M) flows.

| Flow | $m$ | $k$ ($\mu$m$^2$) | $T$ (K) | $h$ (m) | $\tau$ (s) | $P_{in}$ (bar) | $P_{out}$ (bar) | $\chi_{in}$ | $t_r$ (s) |
|------|-----|-----------------|--------|--------|----------|----------------|----------------|------------|----------|
| I    | 0.1 | 1               | 293    | 21     | 0.05     | 10$^{-4}$      | 120            | 60         | 0.45     | 0        |
| M    | 0.35| 0.11            | 300    | 21     | 0.05     | 10$^{-3}$      | 108            | 90         | 0.82     | 1        |

Figure 1. Numerical solution for immiscible N$_2$ and n-C$_8$H$_{18}$ at 0 (black), 0.1 (blue), 7.5 (green), 25 s (red): (a) pressure (□) and gas saturation (△) profiles; (b) amount of N$_2$ (□) and amount of n-C$_8$H$_{18}$ (△) profiles.

While the test is not valuable from physical point of view, it shows the adequateness of the numerical scheme for continuous two-phase flows of compressible components.

4.2. Miscible 2-component fluid

We applied the model from section 2 to a binary mixture of methane CH$_4$ and n-butane n-C$_4$H$_{10}$. The parameters of the test are presented in tables 1 and 2. Dynamic viscosities of the phases $\eta_{ph}$ are approximated using [5]. The boundaries $P_{in}$, $P_{out}$ and $\chi_{in}$ correspond to retrograde area of the mixture.
Figure 2. Miscible CH$_4$ and n-C$_4$H$_{10}$. Propagation of oscillations in terms of concentration of n-butane $Y_2$ (a) and molar fractions of gas phase $G$ and methane $\chi$ (b).

Both phases are presented in the whole space region $[0, L]$ during the experiment, but the liquid phase is immobile at the initial stage due to the relative permeability. The propagation of a wave is shown in figure 2 and is discussed below. Thermodynamics of the mixture forces n-butane concentration $Y_2$ to increase along $x$. It shifts the phase equilibrium in the vicinity of $x \approx 0.2$ m, and the amount of liquid phase grows here causing the decrease of permeability of the whole flow. At the moment around $t \approx 250$ s, the amount of liquid is high enough to move. The mobile portion of the liquid collects the immobile liquid which lies in the front in such manner that the liquid behind the portion can not move. Hence, a new portion of n-butane accumulates near $x \approx 0.2$ m and the described processes repeat.

Figure 3(a) shows oscillations of molar fractions at the right boundary and testifies raised compositions of liquid phase and n-butane in peaks of flow rate [figure 4]. The pressure is not remaining linear but pulses as shown in figure 3(b) for pressure at $x = 0.75$ m. Oscillations at the right boundary have period around 120 s and start at $t \approx 425$ s.

The pulses of pressure and oscillations of the flow rate are in qualitative agreement with an experimental study [1]. The pressure profile $P(x, t = t_j)$ has fissures located at perturbations of $Y_2$. Conducted numerical studies show that replacement of rule (18) for $a_{c,i - 1/2}$ by flow-correct

$$b_{c,i - 1/2} = \frac{2a_{c,i}a_{c,i - 1}}{a_{c,i} + a_{c,i-1}}$$

may cause discontinuities. The effect indicates presence of hyperbolic nature in the studying system and forces to use shock-capturing methods.
Figure 3. Miscible CH$_4$ and n-C$_4$H$_{10}$: (a) oscillations of molar fraction of methane $\chi(L,t)$ (red) and gas phase $G(L,t)$ (black) at the right boundary; (b) oscillations of pressure $P(0.75,t)$.

Figure 4. Miscible CH$_4$ and n-C$_4$H$_{10}$. Oscillations of flux at the right boundary $x = L$.

5. Conclusion
We described analytical and numerical models of miscible and immiscible fluids and implemented them. We conducted numerical experiments for immiscible flow of nitrogen and n-octane, and miscible methane and n-butane. Tests of the model of immiscible components show convenience of chosen numerical scheme in case of two-phase compressible flow. The model of miscible components predicts oscillations of flux at the right boundary and pulses of pressure along
experimental section for a binary mixture of alkanes in retrograde area. The last result in qualitative agreement with an experimental study [1]. We suppose that this approach could model natural gas condensate flows.

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