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# Thermodynamically Consistent Analytical Approach for Streamline Simulations of Multicomponent Hydrocarbon Reservoirs

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# Abstract

One of the most challenging problems for reservoir simulation is the computation of a multicomponent flow of compressible fluids in porous media with mass exchange between phases. In this work, we consider a streamline method for two phase compressible multicomponent flows in hydrocarbon reservoirs. We prove, that even with standard PVT procedures performed at each time step at each spatial point, streamline technology maintain its better scaling ability than traditional finite difference/volume technologies. However, we went further and have treated the thermodynamics in terms of Koldoba & Koldoba approach<sup>7</sup>. The model allows for receiving phase equilibrium curves and other thermodynamic functions in analytical form, thus it achieves the thermodynamic agreement of system and greatly reduces the required computing resources.

#### Introduction

In recent years the streamline simulation methodology has attracted a lot of attention from the research and the oil and gas industry. The reason for this interest lies in the necessity to model detailed reservoir geology. This is motivated, for example, by important applications in gas condensate flows and modeling of CO2 sequestration based on the detailed geological models created by modern modeling tools; such modeling may require large number of computational cells, often several tens millions. In this regard conventional 3D finite difference methods suffer from two drawbacks, numerical smearing and loss of computational efficiency. Finite difference methods based on IMPES approach have the limitation on the time step due to CFL condition in their explicit part. In the case of complex heterogeneous structures of reservoir the smallest cell size defines the time step. This can render the CPU time for simulation impractical. Fully implicit finite difference schemes may use longer time steps but they deal with larger matrixes and in addition may smear the solutions a lot.

The main advantage of conventional streamline methodology is the technique of splitting. First, as in IMPES approach, it solves separately the pressure equation by an implicit method. At this stage one can use rather large time steps. Then the concentrations transportation problem is split again into a series of 1D transport problems. These problems can be solved by any available methods. Because of such splitting the CPU time requirement is significantly reduced.

The developments of streamline method in last decade can be found in a number of papers<sup>2-6,10,12,13</sup>.

Another point in the calculations is the flash procedure. As a rule such specific procedure uses cubic equation of state, like for example Peng-Robinson, for determining thermodynamic characteristics and equilibrium surfaces. This requires the fulfillment of numerous iteration processes during the calculation step and may use a relatively large share of total CPU time consumption. In this paper we propose a special analytic approach in order to reduce the time required for the flash calculations. Coupled with the compositional streamline technique<sup>4</sup> the approach further reduces calculation time and thus facilitates the modeling process for large reservoirs.

Our thermodynamic approach is based on the consideration of Gibb's potentials separately for gas and liquid phases<sup>7</sup>. The form of Gibb's potentials is chosen in such a way that to approximate the equation of state in gas and liquid areas. Then one determines the chemical potentials using conventional thermodynamic relations and obtains the equilibrium surfaces in closed analytic form. Thus our model preserves the thermodynamic consistency and avoids the instabilities connected with the thermodynamic non-consistency. The advantages of such technique lie first of all in significant reduction of computer time consumption because one does not need extensive iteration processes, one uses closed analytic formulas. Another advantage is the calculation with large number of components; this can be also performed rather rapidly because of the analytic nature of thermodynamic relations. The main drawback of the technique is the limitations on pressure and concentrations ranges. Another limitation at the present state of the art is the requirement that the equilibrium surfaces are close to hyperplanes. Here we want to note that many real mixtures have the latter property in real field conditions far from critical thermodynamic parameters. All these we will further improve in the forthcoming papers at the expense of more refined approximations.

## The Compositional Streamline Formulation

In the reservoir modeling the filtration of the components is conventionally described via the system of mass conservation equations

$$\frac{\partial}{\partial t} \left( \phi \sum_{\alpha = o, w, g} x_{i,\alpha} b^{\alpha} s_{\alpha} \right) + \nabla \cdot \left( \sum_{\alpha = o, w, g} x_{i,\alpha} b^{\alpha} \vec{v}_{\alpha} \right) = q_i, \qquad (1)$$
$$i = 1, \dots, N_c.$$

Here subscripts i and  $\alpha$  refer to component and phase respectively. According to Darcy law

$$\vec{v}_{\alpha} = -\frac{K}{\mu_{\alpha}} k_{r\alpha} (s_{\alpha}) (\nabla P - \rho_{\alpha} \vec{g}) .$$
<sup>(2)</sup>

This system should be also closed by normalization conditions

$$\sum_{i=1}^{N_c} x_{i,\alpha} = 1 \quad ; \quad \sum_{\alpha = o, w, g} s_{\alpha} = 1.$$
 (3)

In what follows we do not account for the gravity effects and consider only two phases – oil (liquid) and gas – therefore we omit the gravity summand in (2) and in all sums use  $\alpha = o, g$ . For full description of streamline methodology in compositional case that we are using one can see, for example, Crane et al.<sup>4</sup> and the references therein. All our reasoning remains true for the full system (1)–(3) as well.

The streamline approach is based on the operator splitting concept, which makes possible to consider the pressure evolution separately from the process of concentrations transport. According to this approach and assuming that capillary forces can be neglected one can write the following separate (we suppose that the phases filtration velocities are known, for example, from the previous time layer) equation for the pressure field

$$\phi C_t \frac{\partial P}{\partial t} + \left(\sum_{\alpha=o,g} \vec{v}_{\alpha} c_{\alpha}\right) \cdot \nabla P = -\nabla \cdot \vec{v}_t + Q, \qquad (4)$$

here  $\vec{v}_t = \sum_{\alpha = o,g} \vec{v}_{\alpha}$  and *Q* is source term. The pressure equation

(4) is solved implicitly, and then using formula (2) one can determine the flux  $\vec{v}_t$ , which in turn determines the streamlines. The streamline calculations description can be found in other papers<sup>5,6,8,11</sup>.

Further one should solve the system (1) along all streamlines thus splitting general 3D problem into the series of 1D ones. In order to project the system (1) onto the streamline we first divide our 3D space into the series of streamtubes according to the flux  $\vec{v}_t$ , i.e. each streamline is immersed in some domain along it. As it is conventional in the streamline method we suppose that such stream tubes do not change during the time of concentrations transport.

Let us then integrate equation (1) along the streamtube  $\Omega$  .

Then one has

$$\frac{\partial}{\partial t} \int_{\Omega} \phi \sum_{\alpha=o,g} x_{i,\alpha} b^{\alpha} s_{\alpha} d\Omega + \int_{\partial \Omega} \sum_{\alpha=o,g} x_{i,\alpha} b^{\alpha} \vec{v}_{\alpha} d\partial\Omega = \int_{\Omega} q_i d\Omega.$$
(5)

Remembering our assumption that the streamtube does not change and that there is no flux through the streamtube boundary we have

$$\phi |\Omega| \frac{\partial}{\partial t} \sum_{\alpha=o,g} x_{i,\alpha} b^{\alpha} s_{\alpha} + \int_{A_{2}} \sum_{\alpha=o,g} x_{i,\alpha} b^{\alpha} |\vec{v}_{\alpha}| dA - \int_{A_{1}} \sum_{\alpha=o,g} x_{i,\alpha} b^{\alpha} |\vec{v}_{\alpha}| dA = |\Omega| q_{i}.$$
(6)

Then the simplest discretization of (6) looks as follows providing we take small part of the streamtube

$$\left(\sum_{\alpha=o,g} x_{i,\alpha} b^{\alpha} s_{\alpha}\right)^{n+1} - \left(\sum_{\alpha=o,g} x_{i,\alpha} b^{\alpha} s_{\alpha}\right)^{n} = -\frac{\Delta t}{\phi |\Omega|} \left(\sum_{\alpha=o,g} x_{i,\alpha} b^{\alpha} |\vec{v}_{\alpha}| \cdot |A_{2}| - \sum_{\alpha=o,g} x_{i,\alpha} b^{\alpha} |\vec{v}_{\alpha}| \cdot |A_{1}|\right) + \frac{\Delta t}{\phi} q_{i}.$$
(7)

Solving (7) sequentially for each streamline one determines the saturations and concentrations transport. Then we return to the equation (4) to repeat the process. Let us note that we can also use more general discretization for(5), namely

$$\left(\sum_{\alpha=o,g} x_{i,\alpha} b^{\alpha} s_{\alpha}\right)^{n+1} - \left(\sum_{\alpha=o,g} x_{i,\alpha} b^{\alpha} s_{\alpha}\right)^{n} = -\frac{\Delta t}{\phi |\Omega|} \left(\sum_{j} F_{i;j} A_{j} \vec{n}_{j}\right) + \frac{\Delta t}{\phi} q_{i},$$

where  $F_{i;i}$  is some discretization of the

flux 
$$F_i = \sum_{\alpha=o,g} x_{i,\alpha} b^{\alpha} \vec{v}_{\alpha}$$
;  $A_j$  is the area of appropriate section

and  $\vec{n}_i$  is the unit normal to this section.

# Fast approximation of PVT solver

As it can be seen<sup>4</sup> when applying the streamline methodology in compositional case it is necessary to call many times a PVT procedure in order to perform flash calculations. As a rule such procedure requires involving certain iteration processes that consume much computer time. Below we describe an analytic approach<sup>7</sup> to perform flash procedure, i.e. flash calculations are produced through some explicit analytic formulas. Because of this no iterations are required and much of computer time is saved. Of course suggested analytic formulas have their limitations, which results mainly in the bounded available pressure and concentrations intervals where the approach is applicable.

Let us describe our approach in details. The general idea is to define Gibb's potential separately for gas and liquid phases, then to determine chemical potentials and EOS through differentiation and further in the accordance with the conventional thermodynamics find equilibrium surfaces.

Suppose  $N_i^G$  is a number of particles of component '*i*' in one mole of the gas phase,  $N^G = \sum_i N_i^G$  and  $x_i = N_i^G / N^G$  is the mole concentration of component '*i*' in gas phase. Let us take

Gibbs' potential for gas phase in the form

$$G_G = RT \ln p \sum_i N_i^G + RT \sum_i N_i^G \ln \frac{N_i^G}{N_i^G} + \sum_i N_i^G \chi_i$$

where  $\chi_i(T)$  is some function that depends only on the temperature. The molar Gibbs' potential has the form

$$g_G = RT \ln p + RT \sum_i x_i \ln x_i + \sum_i x_i \chi_i.$$

Further, we can calculate chemical potential for the component k'

$$\mu_{k,G} = \frac{\partial G_G}{\partial N_k^G} = RT \ln \left( p \frac{N_k^G}{N^G} \right) + \chi_k \left( T \right) =$$

$$RT \ln \left( p x_k \right) + \chi_k \left( T \right)$$
(8)

and equation of state for the gas phase

$$V_G = \frac{\partial g_G}{\partial p} = \frac{RT}{p}.$$
(9)

Now suppose similarly that  $N_i^L$  is a number of particles of component 'i' in one mole of the liquid phase,  $N^L = \sum_i N_i^L$  and  $y_i = N_i^L / N^L$  is the mole

concentration of component 'i' in gas phase. Let us take Gibbs' potential for liquid phase in the form

$$G_{L} = RT \ln \left( p + p_{*} \right)^{\alpha} \sum_{i} N_{i}^{L} + RT \sum_{i} N_{i}^{L} \ln A_{i} \frac{N_{i}^{L}}{N^{L}} + \sum_{i} N_{i}^{L} \chi_{i},$$

where again  $\chi_i(T)$  is some function that depends only on the temperature and  $A_i$  are some constants. The molar Gibbs' potential has the form

$$g_L = RT \ln \left( p + p_* \right)^{\alpha} + RT \sum_i y_i \ln A_i y_i + \sum_i y_i \chi_i.$$

Further, we can again calculate chemical potential for the component ' k '

$$\mu_{k,L} = \frac{\partial G_L}{\partial N_k^L} = RT \ln\left(\left(p + p_*\right)^{\alpha} A_k \frac{N_k^L}{N^L}\right) + \chi_k(T) =$$

$$RT \ln\left(\left(p + p_*\right)^{\alpha} A_k y_k\right) + \chi_k(T)$$
(10)

and equation of state for the liquid phase

$$V_L = \frac{\partial g_L}{\partial p} = \frac{\alpha RT}{p + p_*} \tag{11}$$

As it can be seen, the molar volume of liquid phase does not depend on its composition and, see (3.4) in contrast to (3.2), the change in molar density is considered against the reference pressure  $p_*$ , which can be rather high, thus reducing relative change in density with the increase of relative change in pressure. In this sense the liquid phase is low compressible.

Since we know the chemical potentials of the phases, we can calculate phase equilibrium surfaces by the equating of chemical potentials (3.1), (3.3) of each component in different phases. Thus one has

$$A_i y_i = \frac{p x_i}{\left(p + p_*\right)^{\alpha}}.$$
(12)

Coupling of the equations (12) with normalization conditions  $\sum_{i} x_{i} = 1$ ,  $\sum_{i} y_{i} = 1$ ,

the phase equilibrium surfaces in the space of thermodynamic degrees of freedom is obtained. It can be seen from the equations (12) that the K-values  $K_i = x_i / y_i$  do not depend on concentrations and are constants provided constant pressure. Thus proposed model is oriented to such mixtures compositions and ranges of concentrations and pressures where K-values are close to constants and phase equilibrium surfaces are close to hyperplanes.

In order to determine the parameters of our model let proceed in the following way. Let us take some 'base' pressure  $\overline{P}$  and calculate values  $V_L$  and  $dP/dV_L$  for given temperature T and pressure  $\overline{P}$  with the aid of standard Peng-Robinson based procedures. Substituting found values into expression (11) and into expression that is obtained from (11) by differentiating, one determines the parameters  $\alpha$  and  $p_*$ . Then for the same pressure and temperature ( $\overline{P}$  and T) let chose the set of concentrations  $\{c_i\}$  that lies into two-phase domain of concentrations space and for such concentrations let us calculate all pairs  $\{x_i, y_i\}$  again using the standard Peng-Robinson based procedures. Now it is easy to calculate constants  $\{A_i\}$  from equations(12). Let us note that in the methodology we need to use the commercial finite difference based procedure only once in order to get the approximation of the whole range of pressures and concentrations. This is the key point in computer time saving.

Knowing K-values it is possible at once determine the phase

state of the mixture with given overall concentrations  $c_i$  of the components<sup>1</sup>:

- $\sum_{i=1}^{N} c_i K_i < 1$  mixture is in liquid state,
- ∑<sup>N</sup><sub>i</sub> c<sub>i</sub> / K<sub>i</sub> < 1 mixture is in gas state,</li>
   ∑<sup>N</sup><sub>i</sub> c<sub>i</sub>K<sub>i</sub> ≥ 1 and ∑<sup>N</sup><sub>i</sub> c<sub>i</sub> / K<sub>i</sub> ≥ 1 mixture is in two-phase state.

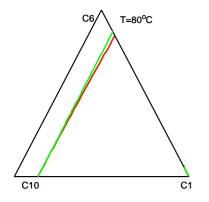
In order to finish thermodynamic calculations when we have the mixture in two-phase state we need to determine one of the saturations, say gas, in the mixture. This can be done by solving the well-known<sup>9</sup> equation for gas saturation S

$$\sum_{i} \frac{c_i(K_i - 1)}{S(K_i - 1) + 1} = 0$$
(13)

It is easy to show that the function with respect to S on the right hand side of equation (13) is monotone with finite numbers of poles. All these poles are located outside the segment [0,1]. Hence the gas saturation can be easily found through the Newton iterations.

#### Test Cases

Numerical experiments show that accuracy of phase equilibrium surfaces obtained via suggested methodology is good enough for cases of closed to constants K-values and for not large pressure differential. Figure 1 demonstrates the phase equilibrium surfaces for 3-components hydrocarbon mixture C1, C6, C10 for two pressures: 40 bars and 50 bars. The temperature is constant and equals 80 °C.



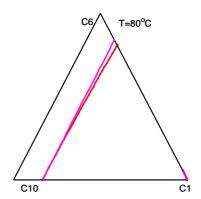
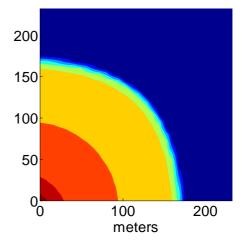


Figure 1: Phase equilibrium surfaces for the mixture C1, C6, C10 with temperature 80 °C and pressure 40 bars (left) and 50 bars (right). The pressure used for approximation is 40 bars. The red curve corresponds to Peng-Robinson equations of state, green and magenta are curves obtained with proposed fast analytic methodology.

To demonstrate the feasibility of fast approximation of PVT solver we compare Compositional Simulator  $(CS)^{15}$  with new flash procedure and Finite Difference Simulator<sup>14</sup>. Along the streamlines the explicit finite differences described above are used. Right now we consider a synthetic model for 4 components mixture C1, C4, C12, C14 with single gas injector and single oil producer. The reservoir is initialized with the concentrations (0.0, 0.1, 0.5, 0.4) which correspond to the oil state under the considered initial pressure 100 bar and temperature 100 °C. A simple well schedule is employed with the production and injection wells maintaining BHP of 60 and 20 bars respectively. Concentrations of the injected mixture are (0.9, 0.1, 0.0, 0.0). Homogeneous media is considered with close to real characteristics and PVT data.

Domain of interest is a 2D rectangular region 240m x 240m, with injector and production wells situated on the diagonal. Figure 2 illustrates the distributions of C1 concentration after 25 days for the grid size 30x30. Figure 3 compares total oil production for FD and CS, results differ less than 3 percents.



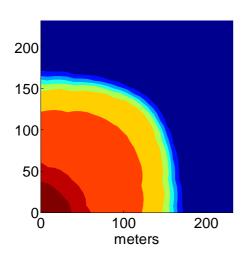


Figure 2: Distribution of C1 concentration after 25 days. Top is FD result and bottom is CS with fast approximation of PVT solver.

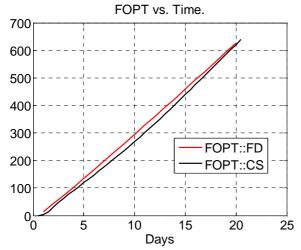


Figure 3: Comparison of Oil Production Total between FD and CS with fast approximation of PVT solver.

The computer time saving due to the fast PVT calculations is about order of magnitude compared with the commercial streamline simulator<sup>4</sup>. We expect even greater performance for the heterogeneous multidimensional problems.

#### Conclusions

We propose new analytic approach to PVT calculations in the framework of of commercial streamline reservoir simulator<sup>15</sup>. Thus in addition to computer time savings provided by streamline methodology we increase the CPU efficiency at the expense of explicit analytic approach for PVT properties.

For geological modeling of hydrocarbon reservoirs we use the compositional streamline simulation models. These detailed models can be very computationally expensive. The efficiency of flash procedures under the conditions of high resolution is extremely significant for the overall performance of the streamline simulator. We compare the developed compositional streamline technique with a finite difference commercial compositional simulator and provide the performance analysis on a number of geological models. It is shown that the combination of high contrast geology and analytical thermodynamic PVT approach leads to significant increase of CPU efficiency.

The drawbacks of proposed thermodynamic approach are: 1) the limitations to pressure and concentrations ranges (in case if Peng-Robinson EOS is taken as reference point), 2) the validity of methodology only in cases when equilibrium surfaces are close to hyperplanes. Nevertheless even with such limitations this model is shown to be useful because, for example, it allows to increase the number of calculation cells in order of magnitude thus allows working with more complex reservoirs models. In addition it allows working with the mixtures with many components that otherwise is very expensive business and also the model provides the way of direct description of field data behavior.

We plan to improve presented PVT methodology at the expense of more refined approximations, separately for gas and liquid phases, to known equations of state.

## Nomenclature

- $\phi$  = porosity
- $b^{\alpha}$  = molar density of  $\alpha$  -th phase (number of moles per unit volume)
- $x_{i,\alpha}$  = molar concentration of *i* -th component in  $\alpha$  th phase (the share of *i* -th component in one mole of  $\alpha$  -th phase)
- $s_{\alpha}$  = saturation (volume share) of  $\alpha$  -th phase
- $\vec{v}_{\alpha}$  = filtration velocity of  $\alpha$  -th phase
- K = permeability
- $\mu_{\alpha}$  = Viscosity of  $\alpha$  -th phase
- $k_{r\alpha}$  = relative permeability of  $\alpha$  -th phase
- $\rho_{\alpha}$  = density of  $\alpha$  -th phase
- $\vec{g}$  = gravity field
- $C_t$  = total compressibility of the fluid
- $c_o$  = phases compressibility of oil phase
- $c_g$  phases compressibility of gas phase
- $p \equiv \text{pressure}$
- T =temperature
- R = the universal gas constant
- $q_i$  = source terms

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