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Numerical Simulation of Multiphase and Multicomponent Fluid Flow in Petroleum Reservoirs Using a Fully Implicit Formulation

Igor V. Lacerda[1], Maria E. S. Galindo[1], Paulo R. M. Lyra[2], Darlan K. E. Carvalho[2]

[1]*Department of Civil Engineering, Federal University of Pernambuco*
Av. Prof. Moraes Rego, 1235 - Cidade Universitária, 50670-901, Recife/PE, Brasil
igor.vasconceloslacerda@ufpe.br
[2]*Department of Mechanical Engineering, Federal University of Pernambuco*
Av. Prof. Moraes Rego, 1235 - Cidade Universitária, 50670-901, Recife/PE, Brasil
Paulo.lyra@ufpe.br, darlan.ecarvalho@ufpe.br

Abstract. Of the many techniques and tools used for estimating oil and gas production in the recovery processes, compositional simulation model is important for problems with complex phase behavior, as in the application of Enhanced Oil Recovery (EOR) methods. The solution of the compositional model involves spatial and time discretization schemes and approaches for handling the coupling of fluid flow and phase behavior. Several solution algorithms arise from combining the different selection of primary variables and decoupling techniques. In this work, we present a Fully Implicit (FI) formulation using cartesian grids for the compositional reservoir simulation based on Equation of State. For the diffusive terms of the equations that describe the mathematical model, we discretize by the Two-Point Flux Approximation (TPFA) finite volume method, while in the advective terms, we apply the first-order upstream weighting. So far, the implemented model considers isothermal flow, up to three-phase flow, and that there is no mass transfer between water and hydrocarbon phases. Physical dispersion and capillary pressure effects are neglected. Our FI formulation is evaluated by solving a benchmark problem found in literature and the results are promising, providing a basis for future implementation of a non-isothermal model to simulate EOR problems, such as steam injection.

Keywords: Petroleum Reservoirs, Compositional Formulation, Fully Implicit Approach.

1 Introduction

Numerical modeling of multiphase and multicomponent fluid flow is an important factor in the oil industry, especially for predicting oil and gas production, allowing field optimization and uncertainty assessment. In this context, efforts have been dedicated to the development of increasingly accurate and physically consistent models (Fernandes et al. [1]). The Black-oil model, widely used in the oil reservoir simulation industry, assumes that the reservoir fluids consist of an explicit water phase and only two hydrocarbon pseudo-components, distributed in an oil phase and a gas phase. The need for compositional models arises especially whenever dealing with volatile oil and gas condensate depletion and with Enhanced Oil Recovery (EOR) process (Chang et al. [2]). In those complex cases, simpler models such as the Black-oil are not suitable.

To numerically solve the large system of nonlinear equations of the compositional models, several approaches are presented in literature, ranging from the choice of primary variables to the level of coupling of the equations. The numerical formulations of reservoir models can be classified as: IMPES (Implicit Pressure, Explicit Saturations), IMPSAT (Implicit Pressure and Saturations), AIM (Adaptive Implicit Method), and FI (Fully Implicit) (Fernandes [3]). Among the Fully Implicit approaches presented in literature, we can highlight two classic formulations: natural variables proposed by Coats [4], and the global variables approach proposed by Collins et al. [5]. In this work, we use the formulation proposed by Collins et al. [5], which uses pressure and global compositions as primary variables. In this formulation, the stability tests and flash procedures are made separately, after computing the primary variables. This decoupling performed by Collins et al. [5] is worthwhile due to the flexibility of having the flash problem completely independent of the material balance equations, allowing a

specific approach to the treatment of fugacity equations (Santos [6]). besides, it allows a quick expansion to non-isothermal problems, one of the future goals to be achieved in this research. In the present paper, we use this formulation with the finite volume method using a Two-Point Flow Approximation (TPFA) scheme for the discretization of the diffusive terms, and the first-order upstream weighting for the advective terms.

2 Mathematical Model

The equations that govern the multiphase and multicomponent fluid flow in porous media are: the equation of the conservation of the mass for the components, the pore volume constraint, the correlations to describe the fluid properties and thermodynamic equilibrium constraints (Fernandes [3], Santos [6]). The phase velocities are evaluated with the Darcy's law. Besides, in this work, we make the following simplifying assumptions: The whole domain is isothermal, there is no mass transfer between the water phase and any of the hydrocarbon phases, local thermodynamic equilibrium is considered and physical dispersion and capillary pressure effects are neglected. The final mathematical model is shown in eq. (1), eq. (2), eq. (3), eq. (4) and eq. (5) below:

$$\frac{1}{V_b}\frac{\partial(N_k)}{\partial t} - \nabla \cdot \sum_{j=1}^{n_p}\left(x_{ij}\xi_j \underset{\sim}{K}\frac{k_{rj}}{\mu_j}(\nabla P - \rho_j g \nabla D)\right) = \frac{\dot{q}_k}{V_b}, \qquad k = 1, \ldots, n_c + 1, \tag{1}$$

$$\sum_{j=1}^{n_p}\frac{n_j}{\xi_j} = V_b\phi, \tag{2}$$

$$f_{k,oil} - f_{k,gas} = 0, \quad k = 1, \ldots, nc, \tag{3}$$

$$\sum_{k=1}^{n_c} x_{kj} = 1, \quad j = 1, \ldots, n_p - 1, \tag{4}$$

$$\sum_{j=1}^{n_p} S_j = 1, \tag{5}$$

where V_b is the bulk volume, N_k is the number of moles of component k, $S_j, \xi_j, \mu_j, k_{rj}, n_j$ and ρ_j are, respectively, the saturation, the molar density, the viscosity, the relative permeability, the number of moles and the mass density of the phase j, x_{kj} and f_{kj} are, respectively, the molar fraction and the fugacity of the component k in the phase j, q_k is the molar rate of the component through the well, $\underset{\sim}{K}$ is the permeability tensor, P is the pressure of the reference phase, taken here as the oil phase, D is the depth, g is the gravity acceleration, ϕ is the porosity, n_p is the number of phases, including water, and n_c is the number of hydrocarbon components present in the system.

Molar, mass densities and fugacity are calculated by the Peng-Robinson Equation of State (Peng and Robinson [7]). To treat the phase appearance and disappearance, the phase stability tests are performed using the stationary point location method (Michelsen [8]), followed by flash calculations, using the Whitson-Michelsen [9] adaptation of the correlations of Rachford-Rice (Rachford and Rice [10]) to include for negative flash calculations.

3 Fully Implicit Formulation

Several numerical formulations are proposed in literature for the solution of the fluid flow model. In this work, we adopt the fully implicit formulation proposed by Collins et al. [4], in which eq. (1) and eq. (2) are solved simultaneously for all control volumes, resulting in a system with $(n_c + 2)n_b$ equations, formed by: $n_c + 1$ mass conservation equations for the hydrocarbon components and water, and a pore volume restriction equation, where n_b is the number of control volumes. We used the Finite Volume Method with Two-Point Flux Approximation (TPFA) to discretize the diffusive terms. For the flux terms, we discretize the advective flow by the first-order upstream weighting. To approximate the permeability terms at every control surface, we use the harmonic mean. Since we are using a fully implicit formulation, for the time integration, we apply the Backward Euler scheme. To solve the nonlinear system, the Newton-Raphson method is implemented. Considering an arbitrary control volume P of a cartesian uniform grid and 1-D fluid flow (x-direction), eq. (1) and eq. (2) can be discretized and written in residual form, as follows:

$$R_k^M = (N_k^{n+1} - N_k^n) - \Delta t \sum_{j=1}^{n_p} \left[F_{kj,e}^{n+1} - F_{kj,w}^{n+1} \right] - \Delta t \dot{q}_{k,}^{n+1}, \quad i = 1, ..., n_c + 1, \tag{6}$$

$$R^V = \sum_{j=1}^{n_p} \frac{n_j^{n+1}}{\xi_j^{n+1}} - V_{b,P} \phi_P^{n+1}, \tag{7}$$

where R_i^M and R^V are the residual of the mass conservation equation of component *k* and of the pore volume constraint, respectively, the superscript n represents the previous time level, n + 1 the current time level and Δt is the time step between the intervals n + 1 and n. In the Fully Implicit method, all properties are evaluated at the current time level. Moreover, $F_{kj,e}^{n+1}$ e $F_{kj,w}^{n+1}$ are the flow of component *k* in phase *j* through the right and left faces, respectively, given by:

$$F_{kj,e}^{n+1} = \left(x_{kj}^{n+1} \xi_j^{n+1} \frac{k_{rj}}{\mu_j} \frac{A}{\Delta x} \underset{\sim}{K} \right)_e \left(P_E^{n+1} - P_P^{n+1} - g \rho_{j,e}^{n+1} (D_E - D_P) \right), \tag{8}$$

$$F_{kj,w}^{n+1} = \left(x_{kj}^{n+1} \xi_j^{n+1} \frac{k_{rj}}{\mu_j} \frac{A}{\Delta x} \underset{\sim}{K} \right)_w \left(P_P^{n+1} - P_W^{n+1} - g \rho_{j,w}^{n+1} (D_P - D_W) \right), \tag{9}$$

where the *E* and *W* subscripts stand for the right and left volumes of the control volume P. Besides, the *e* and *w* subscripts indicate the face shared by the volumes P and E and the volumes W and P, respectively, and A is the face area.

To solve the nonlinear system of equations, the Newton-Raphson method is used considering the pressure and the total number of moles as primary variables, following the approach from Collins et al. [4]:

$$\Delta \vec{X}_l^{n+1} = -\left(\underset{\sim}{J}_l^{n+1} \right)^{-1} \vec{R}_l^{n+1}, \tag{10}$$

where $\Delta \vec{X}_l^{n+1}$ are the changes in the primary variables, $\vec{R}_l^{n+1}$ are the residues and $\underset{\sim}{J}_l^{n+1}$ is the Jacobian matrix at iteration *l*. For a 1D problem, eq. (10) is illustrated below:

$$\begin{bmatrix} \Delta \vec{X}_1^{n+1} \\ \Delta \vec{X}_2^{n+1} \\ \vdots \\ \Delta \vec{X}_{n_b}^{n+1} \end{bmatrix} = - \begin{bmatrix} \underset{\sim}{J}_{1,1}^n & \underset{\sim}{J}_{1,2}^n & \cdots & \underset{\sim}{J}_{1,n_b}^n \\ \underset{\sim}{J}_{2,1}^n & \underset{\sim}{J}_{2,2}^n & \cdots & \underset{\sim}{J}_{2,n_b}^n \\ \vdots & & & \vdots \\ \underset{\sim}{J}_{n_b,1}^n & \underset{\sim}{J}_{n_b,2}^n & \cdots & \underset{\sim}{J}_{n_b,n_b}^n \end{bmatrix}^{-1} \begin{bmatrix} \vec{R}_1^n \\ \vec{R}_2^n \\ \vdots \\ \vec{R}_{n_b}^n \end{bmatrix}, \tag{11}$$

where, an entry (i.e., the submatrix) of the Jacobian matrix for an arbitrary control volume is given by:

$$\underset{\sim}{J}_{i,j} = \begin{bmatrix} \frac{\partial R_i^P}{\partial P_j} & \frac{\partial R_i^P}{\partial N_{1,j}} & \cdots & \frac{\partial R_i^P}{\partial N_{n_c,j}} & \frac{\partial R_i^P}{\partial N_{w,j}} \\ \frac{\partial R_{1,i}^M}{\partial P_j} & \frac{\partial R_{1,i}^M}{\partial N_{1,j}} & \cdots & \frac{\partial R_{1,i}^M}{\partial N_{n_c,j}} & \frac{\partial R_{1,i}^M}{\partial N_{w,j}} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \frac{\partial R_{n_c,i}^M}{\partial P_j} & \frac{\partial R_{n_c,i}^M}{\partial N_{1,j}} & \cdots & \frac{\partial R_{n_c,i}^M}{\partial N_{n_c,j}} & \frac{\partial R_{n_c,i}^M}{\partial N_{w,j}} \\ \frac{\partial R_{w,i}^M}{\partial P_j} & \frac{\partial R_{w,i}^M}{\partial N_{1,j}} & \cdots & \frac{\partial R_{w,i}^M}{\partial N_{n_c,j}} & \frac{\partial R_{w,i}^M}{\partial N_{w,j}} \end{bmatrix}. \tag{12}$$

After solving the system of eq. (10), the primary variables are updated by:

$$\vec{X}_{l+1}^{\,n+1} = \vec{X}_{l}^{\,n+1} + \Delta\vec{X}_{l}^{\,n+1}, \tag{13}$$

then the secondary variables are updated and the process is repeated until convergence is reached in the Newton-Raphson method. After that, the time advance continues until the end of the simulation.

4 Results

In order to evaluate our formulation and verify our implementation, in this section, we present a simulation of the classical two-phase flow problem proposed by Buckley-Leverett [11], which consists of a 1-D flow of water and oil in a petroleum reservoir. Although the system can handle up to three-phases in equilibrium, in this section we describe the solution of the two-phase problem to evaluate a good part of the framework under development, as well as being a problem with a semi-analytic solution. Initially, the reservoir contains 0.2 water saturation and 0.8 oil saturation composed of an n-decane component, with a water injection well at the left extreme side and a production well at the right extreme of the reservoir. The reservoir has a unit dimension L = 1 m along the x-direction, where the flow is considered. The porosity is ϕ = 0.2, the permeability is K_x = 500 mD, the initial pressure is P^0 = 13.79 MPa throughout the reservoir and temperature is constant at 288.71 K, with M = 20 being the mobility ratio between oil and water. Water injection rate is q_w = 2.83e-3 m³/day and the Bottom Hole Pressure (BHP) at the producer well is P_{BHP} = 13.79 MPa. The relative permeability model used was that of Corey [12], whose parameters are shown in Tab. 1, as well as the values of residual saturations. The properties of the n-decane component are shown in Tab. 2.

Table 1. Relative permeability data

Parameter	Nomenclature	Value
End point relative permeabilities	k_{rw}^0 and k_{ro}^0	0.2 and 1.0
Exponents	e_w and e_o	2.0 and 2.0
Residual saturations	S_{wr} and S_{or}	0.2 and 0.35

Table 2. N-decane component data

Property	Value
Critical pressure (MPa)	2.11
Critical temperature (K)	619.28
Critical molar volume (m³/kmol)	0.603
Molar weight (kg/kmol)	142.28
Acentric factor	0.4890

The results of the simulation are obtained for 0.20 Pore Volume Injected (PVI). We compared our solutions with the semi-analytical solution (Buckley-Leverett [11]). Figure 1 shows the convergence study for meshes with 8, 16, 32, 64, 128, 256, and 512 control volumes (CV). We can observe a good agreement with the semi-analytical solution as we refine the mesh, despite the numerical diffusion introduced by the upstream first-order weighting method. In order to evaluate the accuracy of our results, we have used the L1 norm of the error, and as shown in Tab. 3, our implementation converges to the semi-analytical solution. The convergence behavior is illustrated in Fig. 2, where we can observe a good performance compared to linear convergence.

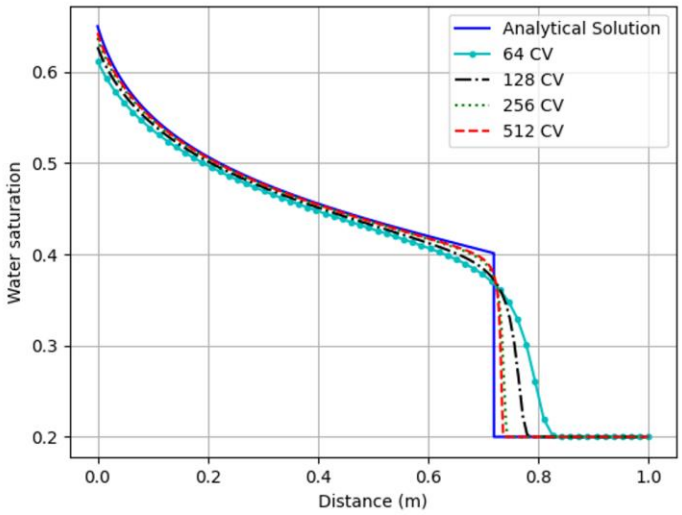

Figure 1. Water saturation obtained for the FI method compared to the semi-analytical solution

Table 3. Error norm and convergence rates

Control volumes	$L_{1_{error}}$	$L_{1_{rate}}$
8	0.06308	-
16	0.04842	0.3816
32	0.03020	0.6809
64	0.01938	0.6399
128	0.01181	0.7148
256	0.00529	1.1572
512	0.00386	0.4559

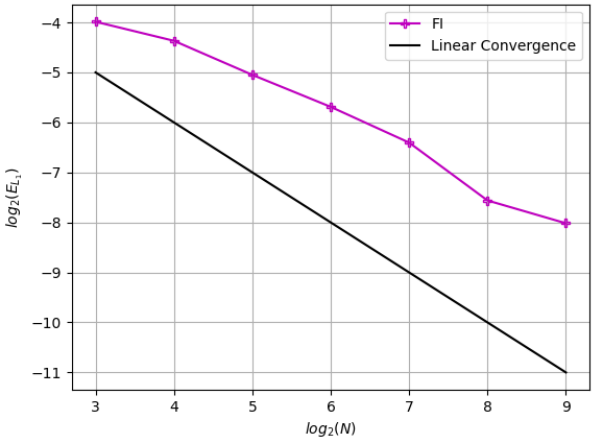

Figure 2. Error norm variation with number of cells

5 Conclusions

In the present work, we show a FI formulation proposed by Collins et al. [5] for modeling compositional flow in petroleum reservoirs, based on the Equation of State of Peng and Robinson [7], which uses pressure and global compositions as primary variables. To validate our formulation and assess its accuracy, we compared our results with the semi-analytical solution of a classical problem in literature. Our results are very promising and in the near future we intend to apply them to more complex problems, simulate two-dimensional problems, and implement the non-isothermal model to simulate Enhanced Oil Recovery problems, such as steam injection, using a novel method for the flash calculations proposed in literature. Furthermore, in the long term, we intend to extend this work to general polygonal and polyhedral unstructured meshes.

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