XLI CILAMCE
XLI Ibero-Latin American Congress on Computational Methods in Engineering
16-19 November, 2020 FOZ DO IGUAÇU PARANÁ - BRAZIL

Numerical Simulation of Multiphase and Multicomponent Fluid Flow in Petroleum Reservoirs Using an IMPEC Compositional Formulation and a Second Order MUSCL Type Finite Volume Method

Maria E. S. Galindo[1], Darlan K. E. Carvalho[1]

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

Abstract. The numerical modeling of multiphase and multicomponent fluid flow in petroleum reservoirs is extremely complex and computationally demanding. Frequently, simpler black-oil models are not suitable for cases in which the reservoir fluid is volatile and composed by several pseudo-components with distinct characteristics. For those cases, the use of a compositional simulation based in Equations of State (EOS) is of utmost importance. In this work, we present an Implicit Pressure Explicit Composition (IMPEC) formulation using cartesian grids for the compositional reservoir simulation based on an EOS approach. Diffusive terms in flux and transport equations are discretized by the Two-Point Flux Approximation (TPFA) finite volume method. Besides, to improve front resolution and accuracy, we discretize the advective terms of the transport equations by the second-order Monotonic Upstream-centered Scheme for Conservation Laws (MUSCL) method. 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 is neglected. Our IMPEC formulation is evaluated by solving a benchmark problem found in literature. The accuracy of our approach is evaluated comparing our results with those obtained by a commercial reservoir simulator (CMG-GEM).

Keywords: Petroleum Reservoirs, Compositional Formulation, Implicit Pressure Explicit Composition (IMPEC) Approach, Monotonic Upstream-centered Scheme for Conservation Laws (MUSCL)

1 Introduction

The numerical modeling of the multiphase and multicomponent fluid flow in heterogeneous petroleum reservoirs is extremely complex and computationally demanding. The Black-oil model, a simpler compositional model vastly used in the petroleum reservoir simulation industry, assumes that the reservoir fluids consists of one explicit water component and phase and only two hydrocarbon pseudo-components, distributed in one oil phase and one gas phase. For that reason, Black-oil models are not suitable for cases where the reservoir fluid is composed by several pseudo-components with distinct characteristics, the fluid composition varies along the reservoir or in processes where Enhanced Oil Recovery (EOR) techniques are applied, such as polymer injection, thermal recovery, Water Alternate Gas (WAG), etc. The importance of the compositional effects present in those cases, raise the need for more complex compositional models, such as EOS based compositional models, that are capable of properly describe the complex phase behavior.

The numerical simulation of the compositional effects involves the solution of a system of non-linear equations that comprises the mass conservation, the Darcy law for each phase and fugacity constraints. Several approaches to solve this system are presented in literature, varying from the choice of the primary variables to the coupling level of the system of equations. In this work, we have used the classical IMPEC approach, proposed by Ács et. al.[1], in which the pressure field is computed implicitly and the compositions are computed explicitly. In this formulation the stability tests and flash procedures are made separately, after computing the overall system composition. The pressure equation is discretized by the finite volume method using a Two-Point Flux Approximation (TPFA) scheme. Besides, in order two improve front resolution and accuracy, the second order MUSCL-type approach of Van Leer (Moshiri and Manzari [2]) is used to solve the composition equations, where monotonicity is guaranteed by the use of the Van Leer's slope limiter.

2 Mathematical Model

In this paper, we have used a model that arises from the proper application of the following relations: material balance equations, correlations to describe the fluid properties and thermodynamic equilibrium constraints (Fernandes [3]). Those form a system of $(n_p - 1)n_c + n_p + 1$ equations and unknowns, where n_p is the number of phases, including water, and n_c is the number of hydrocarbon components present in the system (Schmall [4]). In this work, we make the following simplifying assumptions: the flow is isothermal, there is no mass transfer between the water phase and the hydrocarbon phases, physical dispersion and capillary pressure effects are neglected. In this context, the final mathematical model is shown in eq. (1) to eq. (4) given bellow:

$$\frac{1}{V_b}\frac{\partial N_k}{\partial t} = \frac{1}{V_b}\sum_{j=1}^{n_p}\vec{\nabla}\cdot\left(x_{kj}\xi_j\frac{k_{rj}}{\mu_j}\underset{\sim}{K}\cdot(\nabla P + \rho_j g\nabla D)\right) + \frac{q_k}{V_b}, \quad k = 1,..n_c + 1, \tag{1}$$

$$f_{k,oil} - f_{k,gas} = 0, \quad k = 1, ..., n_c, \tag{2}$$

$$\sum_{k=1}^{n_c} x_{kj} = 1, \quad j = 1...n_p - 1, \tag{3}$$

$$\sum_{j=1}^{n_p} S_j = 1, \tag{4}$$

where V_b is the bulk volume, N_k is the number of moles of component k, S_j, ξ_j, μ_j, k_{rj} and ρ_j are, respectively, the saturation, the molar density, the viscosity, the relative permeability 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 and g is the gravity acceleration.

Molar, mass densities and fugacities are calculated in this work by the Peng-Robinson's model (Peng and Robinson [5]). For the phase appearance and disappearance treatment, phase stability tests are performed using the stationary point location method (Michelsen [6]), followed by flash calculations, using Whitson-Michelsen's [7] adaptation of the Rachford-Rice correlations to include negative flash calculations.

3 IMPEC Formulation

Several numerical formulations were proposed in literature for the solution of the fluid flow model. In this work, we have chosen the IMPEC formulation based on Ács et. al. [1] due to its simplicity and easy implementation when compared to others formulations. In the approach proposed by Ács et. al. [1], the pressure equation is obtained from the equality between the pore volume, V_p and the total volume occupied by the reservoir fluid, V_t:

$$V_p(P) = V_t(P, N_1, ...N_{n_c+1}). \tag{5}$$

After some algebraic manipulation of eq. (5) and eq. (1), the pressure equation has the following form (Fernandes [3]):

$$\left(\phi_0 C_f - \frac{1}{V_b}\frac{\partial V_t}{\partial P}\right)\frac{\partial P}{\partial t} = \sum_{k=1}^{n_c+1}\frac{\partial V_t}{\partial N_k}\left[\sum_{j=1}^{n_p}\vec{\nabla}\cdot\left(x_{kj}\xi_j\frac{k_{rj}}{\mu_j}\underset{\sim}{K}\cdot(\nabla P + \rho_j g\nabla D)\right) + \frac{q_k}{V_b}\right], \tag{6}$$

where C_f is the rock compressibility and ϕ_0 is the rock porosity taken at a reference pressure. The total volume partial derivative terms are computed using the Peng-Robinson EOS [5]. The pressure equation is solved implicitly. From the initial water saturation, reservoir fluid composition and pressure distribution, the IMPEC formulation, consists in: 1. Compute pressure implicitly by eq. (6); 2. Compute fluxes using Darcy's Law; 3. Compute composition explicitly by eq. (1); 4. Update global composition; 5. Perform the phase stability test and the flash calculations; 6. If the simulation time does not reach the final time, advance in time and go to step 1. Otherwise, stop the simulation and exit. In the following section we present the numerical finite volume formulation used to discretize the partial differential equations of the IMPEC formulation. For the approximation of the diffusion terms present in these equations, we have used the classical linear second order Two Point Flux Approximation (TPFA) method. For the transport terms, we have used a second order accurate MUSCL-type finite volume method. Finally, we have applied the first order Euler method for the time discretization and compared our results against the solution obtained by the commercial reservoir simulator GEM from CMG [8].

3.1 Approximate Pressure Equation: The TPFA method

Considering an arbitrary control volume of a cartesian uniform grid and 1-D fluid flow (x direction), the approximated pressure equation can be obtained by applying the TPFA method for that grid block, as follows:

$$\left(V_b\phi_0 C_f - \frac{\partial V_t^n}{\partial P}\right)_M \frac{P_M^{n+1} - P_M^n}{\Delta t} = \frac{V_{t,M}^n - V_{p,M}^n}{\Delta t} + \sum_{k=1}^{n_c+1} \frac{\partial V_{t,M}^n}{\partial N_{k,M}} \left[\sum_{j=1}^{n_p} \left[\left(x_{kj}\xi_j\lambda_{rj}\frac{2AK_x}{\Delta x}\right)_l (P_L^{n+1} - P_M^{n+1}) - \left(x_{kj}\xi_j\lambda_{rj}\frac{2AK_x}{\Delta x}\right)_r (P_M^{n+1} - P_R^{n+1})\right] + q_k\right], \tag{7}$$

where $\lambda_{rj} = k_{rj}/\mu_j$, the n superscript indicates the time step, the L and R subscripts stands for the left and right volumes of the analyzed control volume, M. Besides, the l and r subscripts indicates the face shared by the volumes L and M and the volumes M and R, respectively, and A is the face area. The $(V_{t,M}^n - V_{p,M}^n)$ term in the right side of the pressure equation is a correction term for the truncation errors associated to the linear approximations made to obtain eq. (6). For more details regarding how this term arises see Ács et. al. [1]. The fluid properties at the control surfaces of the grid blocks were approximated by weighted arithmetic average of the neighboring cells values.

3.2 Approximate Component Transport Equation: The MUSCL method

For the discretization of the advective terms present in the composition equation, we have used the second order Monotonic Upstream-centered Scheme for Conservation Laws (MUSCL) method. This approach consists in reconstructing the desired variable at each control volume (Galidez-Ramirez et. al. [9]). As a second-order polynomial reconstruction is used, a linear reconstruction is determined from the mean values of the two closest neighboring volumes. After the linear reconstruction at each volume, the property is extrapolated at the left and right sides of each grid block interface. In order to reinforce monotonicity, a slope limiter must be used in this process. The procedure to obtain the number of moles using a second order approximation at the interfaces is shown in eq. (8) and eq. (9) bellow (Moshiri and Manzari [2]),

$$N_{k_{i+1/2}}^- = N_{ki} + 0.5Lim(r_{k_{i-1/2}}^+)(N_{ki} - N_{ki-1}), \tag{8}$$

$$N_{k_{i+1/2}}^+ = N_{ki+1} - 0.5Lim(r_{k_{i+3/2}}^+)(N_{ki+2} - N_{ki+1}), \tag{9}$$

where the subscript $i + 1/2$ represents that the property is calculated at a interface, while i plus an integer value, represents that the property is taken at a grid volume. Also, the plus(+) and minus(-) superscripts indicates the right and left extrapolated states of the interface, respectively, r is the ratio of gradients and Lim is the slope limiter. Here, we have used the Van Leer slope limiter, given by:

$$Lim_{VanLeer} = \frac{r + |r|}{r + 1}. \tag{10}$$

After the reconstruction, we compute the component flux at the interface by using the Local Lax-Friedrichs (LLF) scheme (Moshiri and Manzari [2]), which is given by,

$$F_{ki+1/2} = \frac{1}{2}\left(F_{k_{i+1/2}}^+ + F_{k_{i+1/2}}^- - |\alpha_{LLF}|(N_{k_{i+1/2}}^+ - N_{k_{i+1/2}}^-)\right), \tag{11}$$

where, α_{LLF} is the maximum eigenvalue of the hyperbolic system, representing the maximum wave velocity. This parameter can be calculated as follows:

$$|\alpha_{LLF}| = max(|{\alpha_-}^{max}|, |{\alpha_+}^{max}|, |{\alpha_{G-}}^{max}|, |{\alpha_{G+}}^{max}|, |{\alpha_m}^{max}|), \tag{12}$$

where α_- is evaluated at N_{k-}, α_+ at N_{k+}, α_m is evaluated at $N_{km} = \frac{N_{k-}+N_{k+}}{2}$ and α_{G-} and α_{G+} are the eigenvalues corresponding to the Gauss points at $N_{km} + \frac{N_{k-}-N_{km}}{\sqrt{3}}$ and $N_{km} + \frac{N_{k+}-N_{km}}{\sqrt{3}}$, respectively.

4 Results

In order to evaluate our formulation and verify our implementation, we present a problem involving the multicomponent, three phase and 1-D flow of water, oil and gas in a petroleum reservoir that was adapted from a 3-D problem presented in Schmall [4]. In this example, we have a water injection well at the left extreme side of the reservoir and a production well at the right extreme side. The reservoir has the dimensions of $2731.2m \times 10.67m \times 10m$ and the flow is along the x-direction. The porosity is $\phi_0 = 0.35$, the permeability is $K_x = 10mD$, the initial water saturation is $S_w^0 = 0.3$, which is equal to the water critical saturation, temperature is $T = 344.25K$ and the initial pressure is $P^0 = 10.34MPa$ throughout the reservoir. Oil residual saturation is $S_{or} = 0.1$, water injection rate is $q_w = 35.75m^3/day$ and the Bottom Hole Pressure (BHP) at the producer well is $P_{BHP,prod} = 8.96MPa$. The initial fluid composition at the reservoir is: $z_{C1} = 0.5$, $z_{C3} = 0.03$, $z_{C6} = 0.07$, $z_{C10} = 0.2$, $z_{C15} = 0.15$, $z_{C20} = 0.05$, where z is the global composition. The results were obtained after 200 days of simulation. We used a CFL of 0.5. We have compared our solutions with the ones obtained by the GEM simulator from Computer Modeling Group [8] with a mesh of 1024 control volumes (CV). In order to evaluate the accuracy of our formulation we have used the L_2 norm of the error. Table 1 shows the error norm and convergence rates, where we can notice the best accuracy of the MUSCL method when compared to the FOUM (First Order Upwind Method). The error behaviour for the L_2 norm is shown in Fig. 1, where we can see that the MUSCL method has a slightly uneven behaviour. This can be explained by the slope limiting process required in high order methods to preserve monotonicity at the shock front. This process, however, can contaminate the solution in smooth regions behind of the shock, deteriorating the optimal order of accuracy at the discontinuity (Galindez-Ramirez et. al. [9]).

Table 1. Error norm and convergence rates

	FOUM		MUSCL	
Cells	L_{2error}	L_{2rate}	L_{2error}	L_{2rate}
8	0.07439	-	0.07974	-
16	0.05772	0.3659	0.04599	0.7939
32	0.04165	0.4708	0.03146	0.5481
64	0.02688	0.6316	0.01559	1.0126
128	0.02132	0.3345	0.01032	0.5949
256	0.01913	0.1562	0.00631	0.7103

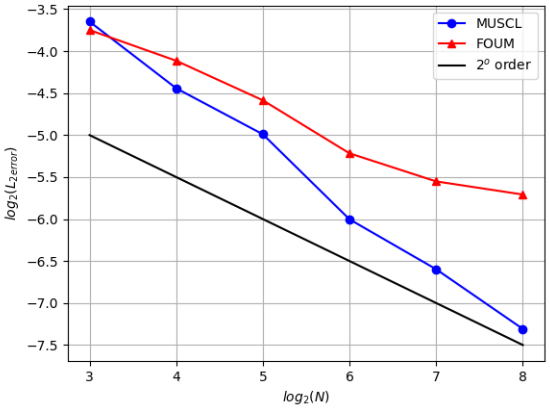
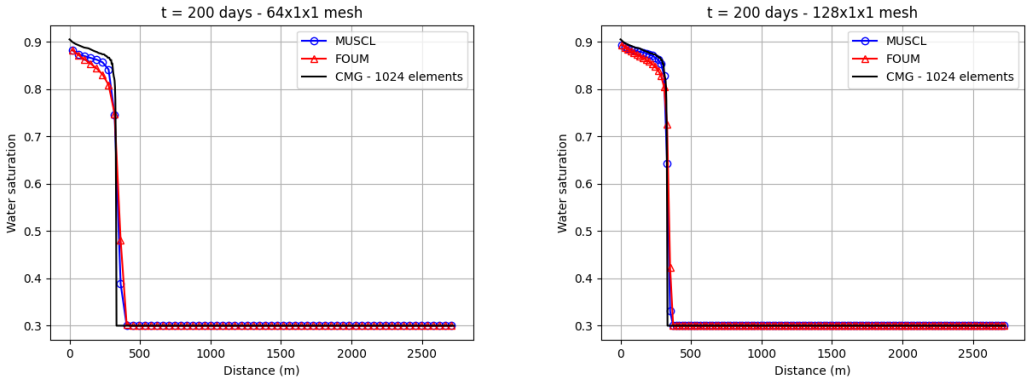


Figure 1. Error norm variation with number of cells

The more accurate solution of the MUSCL method can also be seen in the Fig 2.

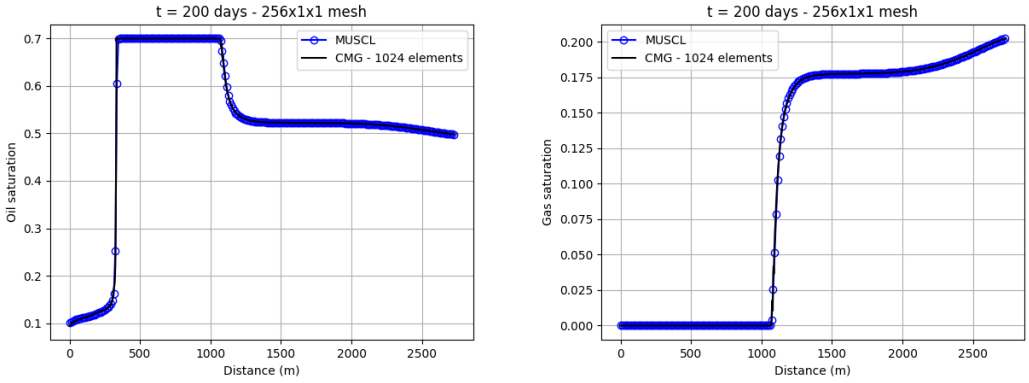


(a) 64 control volumes

(b) 128 control volumes

Figure 2. Water Saturation solution obtained for the MUSCL method and FOUM with a) 64 CV and b) 128 CV

In Fig. 3, we present the oil saturation and the gas saturation profiles using our higher order method for a mesh with 256 CV against the reference solution obtained by the CMG-GEM software for a mesh with 1024 CV.



(a) Oil saturation profile

(b) Gas saturation profile

Figure 3. Results of three-phase six component problem after 200 days of simulation using a 256 CV mesh

5 Conclusions

In this work, we present an IMPEC formulation for the modeling of compositional flows in petroleum reservoirs. The transport problem is solved through the higher order MUSCL method using the LLF approach. To evaluate the accuracy of our formulation, we have compared our results with the FOUM method and the results obtained by CMG-GEM software. Our results are very promising and in the future, we will use a more accurate Riemann solver and the IMPSAT (Implicit Pressure and Saturation) formulation to handle more complex problems.

Acknowledgements. We would like to thank CNPq (Conselho Nacional de Desenvolvimento Científico e Tecnológico) for the financial support and the PADMEC group (Processamento de Alto Desempenho em Mecânica Computacional).

Authorship statement. The authors hereby confirm that they are the sole liable persons responsible for the authorship of this work, and that all material that has been herein included as part of the present paper is either the property (and authorship) of the authors, or has the permission of the owners to be included here.

References

[1] Ács, G., Doleschall, S., & Farkas, E., 1985. General purpose compositional model. *SPE Journal*, vol. 25(4), pp. 543–553.
[2] Moshiri, M. & Manzari, M. T., 2019. A comparative study of explicit high-resolutions schemes for compositional simulations. *International Journal of Numerical Methods for Heat and Fluid Flow*, vol. 29, pp. 94–131.
[3] Fernandes, B. R. B., 2014. Implicit and semi-implicit techniques for the compositional reservoir simulation based on volume balance. Master's thesis, The University of Texas at Austin, Austin, United States.
[4] Santos, L. O. S., 2013. *Development of a Multi-Formulation Compositional Simulator*. PhD thesis, The University of Texas at Austin, Austin, United States.
[5] Peng, D. Y. & Robinson, D. B., 1976. A new two-constant equation of state. *Industrial and Engineering Chemical Fundamentals*, vol. 15(1), pp. 59–64.
[6] Michelsen, M. L., 1982. The isothermal flash problem. Part I: Stability. *Fluid Phase Equilib.*, vol. 9(1), pp. 1–19.
[7] Whitson, C. H. & Michelsen, M. L., 1989. The negative flash. *Fluid Phase Equilibr.*, vol. 53, pp. 51–71.
[8] CMG, 2019. *CMG User Guide 2019*. Computer Modelling Group Ltd, Calgary, Alberta, Canada.
[9] Galindez-Ramirez, G., Carvalho, D. K. E., & Lyra, P. R. M., 2020. Numerical simulation of 1-D oil and water displacements in petroleum reservoirs using the correction procedure via reconstruction (CPR) method. *Computational Geosciences*, vol. 24, pp. 1–15.