Three-Dimensional Multiphase Flow Simulation in Petroleum Reservoirs using the Mass Fractions as Dependent Variables

Abstract
This paper describes a numerical methodology for solving three-dimensional multiphase flow in petroleum reservoirs. The mathematical model encompasses the Darcy’s equations and the mass conservation equation for the oil, gas and water components. To account for the gas phase appearance/disappearance, without employing special strategies, the method uses the mass fractions as dependent variables. The mathematical model uses boundary-fitted coordinates which permits to deal with complex reservoir boundaries and offers the opportunity of better representing curvilinear geological structures. The solution is fully implicit and includes the proposition of a well model for non-orthogonal discretization.

Introduction
The simulation of the multiphase flow of oil, gas and water in porous media are usually carried out using the saturation and pressure as dependent variables. However, there are thermodynamic conditions in petroleum reservoirs in which the gas is dissolved in the oil, but the gas phase is absent. Since the saturation is related to the existence of the phase, when the gas phase disappears, but the gas component is still present in the oil phase, the numerical scheme must take into account the phase appearance/disappearance. To deal with this problem it is necessary to change the variables during the simulation, or to avoid the phase disappearance, keeping a residual value for the saturation. These strategies poses numerical difficults and may cause instabilities during the solution procedure.

One alternative for by-passing this problem is to use the mass fractions of the components as dependent variables, as done in Prais and Campagnolo [1] and Britto [2]. This guarantees that, in the case of the gas phase disappearance, the mass fraction of the gas component, representing the total mass of gas dissolved in the other phases, will be non-zero.

This paper presents a numerical method for solving 3D multiphase flow of oil, water and gas in complex reservoirs using the mass fractions as dependent variables and a fully implicit formulation. For handling the complex geometries of the reservoirs, a non-orthogonal boundary-fitted coordinate system is used. This type of structured discretization has been previously used by Maliska et al [3,4] for modeling two and three phase flows with IMPES formulation. Curvilinear orthogonal grids have been used in the past by Hirasaki and O’Dell [5], Sharp and Anderson [6] and Robertson and Woo [7] among others.

The model is applied to solve three-dimensional two-phase and three-phase flows in petroleum reservoirs.

Problem Formulation
For petroleum reservoirs with heavy or low volatile oils, the black-oil model is largely used. To obtain the governing equations the mass balance for each component, oil water and gas, is performed. The governing equations are

$$\frac{\partial}{\partial t}(\phi \rho z^w) = \nabla \cdot \left( \lambda \nabla \Phi^w \right) - m^w$$  (1)
\[ \frac{\partial}{\partial t} \left( \phi \rho^w z^w \right) = -V \left[ x^{\omega} \lambda^\omega \nabla \Phi^\omega \right] - x^{\omega} m^\omega \]  

(2)

\[ \frac{\partial}{\partial t} \left( \phi \rho^g z^g \right) = -V \left[ \left(1 - x^{\omega} \right) \lambda^g \nabla \Phi^g + \lambda^g \nabla \Phi^g \right] - \left(1 - x^{\omega} \right) m^g - m^g \]  

(3)

where \( \phi, \lambda, x^\omega, z^\omega, \Phi, \rho^w \), are the porosity, permeability, mass fraction of the oil component in the oil phase, global mass fraction of component \( c \), phase potential and average density of the mixture, respectively. Inspecting Eqs. (1) to (3) one can see that the mass fractions \( z^\omega \), \( z^g \) and \( z^s \) and the phase potentials are unknowns. The phase potentials can be related to the oil pressure and capillary pressures by

\[ \Phi^\omega = p^\omega + \gamma^\omega z^\omega \]  

(4)

\[ \Phi^g = p^g - p^{cw} + \gamma^g z^g \]  

(5)

\[ \Phi^s = p^s + p^{cs} + \gamma^s z^s \]  

(6)

Replacing the phase potentials by the above expressions, the unknowns of the equation system become the mass fractions and the oil pressure. Therefore, it is needed a closure equation. In this case the global mass (oil + gas + water) is invoked. This is expressed by

\[ z^\omega + z^g + z^s = 1 \]  

(7)

In spite of having a well-posed problem, Eqs. (1) to (3), restricted to Eq. (7), do not form an appropriate equations system to be solved by iterative methods. To obtain \( z^\omega, z^g \) and \( z^s \) such that Eq.(7) is conserved would require the creation of a correction equation to advance one of the mass fractions based on the error of the global mass conservation. Therefore, it is preferable to satisfy Eq. (7) summing up Eqs. (1) to Eqs. (3), and discarding the mass conservation for the gas component, Eq. (3). Using this procedure one finds the global mass conservation equation, given by

\[ \frac{\partial}{\partial t} \left( \phi \rho^w \right) = -m^w - m^\omega - m^g \]  

+ \[ V \left[ \lambda^\omega \nabla \Phi^\omega + \lambda^g \nabla \Phi^g + \lambda^s \nabla \Phi^s \right] \]  

(8)

The unknowns are then the mass fractions of oil and water and the oil pressure, since the phase potentials are related to the oil pressure and capillary pressures through Eqs.(4-6). The corresponding equation system to be solved is, therefore, formed by Eqs. (1) and (2) and Eq. (8).

**Transformed and approximate equations**

The equation system is solved using the fully implicit formulation with Newton’s method in a generalized curvilinear coordinate framework. Two approaches can be used to obtain the approximate equations. To integrate the conservation equations in the irregular volumes or to transform the conservation equations to the new coordinate system. The latter approach is used in this work, what consists in transforming the governing equations to the new \( (\xi, \eta, \gamma) \) system and then integrate the transformed equation in a regular domain, as described in Maliska [9]. To illustrate, the transformed equation for the water component, Eq. (9), is taken as example and written below as

\[ \frac{1}{J} \frac{\partial}{\partial \xi} \left[ \phi \rho^w \right] + \frac{m^w}{J} = \]  

\[ \frac{\partial}{\partial \xi} \left[ D^w \frac{\partial \Phi^w}{\partial \xi} + D^w \frac{\partial \Phi^w}{\partial \eta} + D^w \frac{\partial \Phi^w}{\partial \gamma} \right] + \]  

\[ \frac{\partial}{\partial \eta} \left[ D^w \frac{\partial \Phi^w}{\partial \xi} + D^w \frac{\partial \Phi^w}{\partial \eta} + D^w \frac{\partial \Phi^w}{\partial \gamma} \right] + \]  

\[ \frac{\partial}{\partial \gamma} \left[ D^w \frac{\partial \Phi^w}{\partial \xi} + D^w \frac{\partial \Phi^w}{\partial \eta} + D^w \frac{\partial \Phi^w}{\partial \gamma} \right] \]  

(9)

The equations for the oil component and for pressure are similar and are not presented here. The finite-volume method, which consists in integrating the conservation equations in their divergence form, is used. Integration of Eq.(9) in time and in space, Fig.1, results
The derivatives are evaluated using central differencing using the available neighboring control volumes. If and orthogonal grid is used seven control volumes are involved in the direct derivatives calculation, originating a 7-diagonal blocked matrix to be solved. For a non-orthogonal grid, in the other hand, 19 control volumes are required for calculating the direct and cross-derivatives. The resulting blocked matrix contains, therefore, 19-diagonals, in which each entry is a 3x3 matrix. For example, the direct derivative of $\phi$ and the cross derivative of $\phi$ with respect to $\eta$ at the east face of a control volume are given by

$$\left( \frac{\partial \phi}{\partial \xi} \right)_e = F_e \left[ \frac{\Phi_e - \Phi_p}{\Delta \xi} \right]$$

and

$$\left( \frac{\partial \phi}{\partial \eta} \right)_e = \frac{F_e}{F_e} \left[ \frac{F_{p\Phi_s} \Phi_{p\Phi_e} + F_{p\Phi_p} \Phi_{p\Phi_e} + F_{p\Phi_N} \Phi_{p\Phi_e} + F_{p\Phi_s} \Phi_{p\Phi_N} + F_{p\Phi_p} \Phi_{p\Phi_N} + F_{p\Phi_N} \Phi_{p\Phi_N}}{F_e} \Delta \eta \right]$$

The F's are called the fault coefficients and they allow that only one approximate equation represents all control volumes (interior and boundaries). The use of the F’s coefficients allows also the simulation of reservoirs with geological faults, by specifying a distribution of F’s, which specifies no-flow at the fault’s boundaries. The use of these coefficients simplifies enormously the derivation of the approximate equations for different boundary conditions and fault distribution.

Details of the derivation of these coefficients and the integration of the other conservation equations can be found in [8].

**Numerical Strategy.** If one is seeking for a fast algorithm, it is not feasible to keep the 19 control volumes implicitly in the solution procedure. Recalling that twelve of the matrix diagonals are due to the non-orthogonality of the grid, it is possible to keep the entries of those diagonals at low values, if a quasi-orthogonal grid is constructed, and identically zero if a orthogonal mesh is used. Therefore, in order to built a scheme which resembles the one constructed using orthogonal grids, that is, with 7-diagonals, one can collect the non-orthogonal terms and add them to the independent term of the equation. Using this strategy these terms are kept constant during one or more Newton’s iteration, depending on the sensitivity of the equations system to convergence. It must be pointed out that this procedure solves the approximate equations exactly, and the influence of putting the non-orthogonal terms in the right-hand side of the equations may only be in the convergence rate of the algorithm. Since petroleum reservoirs are usually thin with respect to the horizontal area, it is not difficult to create quasi-orthogonal grids. This would keep the influence of the non-orthogonal terms over the convergence rate to a minimum. Studies are now been undertaking to analyze how severe can be the non-orthogonality of the grid, still keeping the robustness of the method.

**Well Model.** Since the grid blocks are many times larger than the well size, it is necessary to express the mass flow rate of the well as function of the well pressure, at same vertical position, and the corresponding pressure of the control volume at that same position. Using appropriate flow equations for the flow inside the well it is possible to relate the well pressure, at the same vertical position, to the bottom well pressure. In this section it is developed a well model for non-orthogonal grids. Using the well known procedure for determining the equivalent wellblock radius[10] one obtains
\[ P_P = P_F^* + \frac{m\mu}{2kh\rho\pi} \ln \left( \frac{r_0^w}{r_0^w} \right) \]  

(13)

Considering Fig. 2, and applying Eq. (13) one obtains

\[ P_E - P_P = \frac{m}{2h\lambda\pi} \ln \left( \frac{d_E}{r_0^w} \right) \]  

(14)

\[ P_W - P_P = \frac{m}{2h\lambda\pi} \ln \left( \frac{d_W}{r_0^w} \right) \]  

(15)

\[ P_N - P_P = \frac{m}{2h\lambda\pi} \ln \left( \frac{d_N}{r_0^w} \right) \]  

(16)

\[ P_S - P_P = \frac{m}{2h\lambda\pi} \ln \left( \frac{d_S}{r_0^w} \right) \]  

(17)

Performing a mass balance over the control volume centered at \( P \) one obtains

\[ \lambda G_{1e} (P_E - P_P) - \lambda G_{1w} (P_F - P_W) + \lambda G_{5n} (P_N - P_P) - \lambda G_{5s} (P_P - P_S) = m \]  

(18)

where the \( G_{i,j} \) are metric coefficients involving only geometric parameters from the coordinate transformation.

Substituting in Eq. (18) the pressure differences by their logarithmic expressions one gets

\[ -2h\pi + \lambda G_{1e} \ln \left( \frac{d_E}{r_0^w} \right) - \lambda G_{1w} \ln \left( \frac{d_W}{r_0^w} \right) + \lambda G_{5n} \ln \left( \frac{d_N}{r_0^w} \right) - \lambda G_{5s} \ln \left( \frac{d_S}{r_0^w} \right) = 0 \]

(19)

After some algebraic manipulation the equivalent wellblock radius is found as

\[ r_0^* = \left[ e^{-2h\pi} d_E G_{1e} d_W G_{1w} d_N G_{5n} d_S G_{5s} \right]^{\beta} \]  

(20)

where

\[ \beta = \left( G_{1e} + G_{1w} + G_{5n} + G_{5s} \right)^{-1} \]  

(21)

For a Cartesian grid the above expression furnishes the well known expression

\[ r_0^* = 0.208 \Delta x \]  

(22)

Knowing \( r_0^* \) the W1 (well index) can be calculated and the relation between the well pressure and the grid block pressure is established for general non-orthogonal grids.

The model described in this work also includes the implicit treatment of the wells for well conditions of prescribed well bottom pressure, mass flow of water, oil and gas, and global mass flow at standard conditions.

**Solution Method.** The residual equations for the conservation of oil and water and for the global conservation are expanded according to

\[ \left( F_x^k \right)^{k+1} = \left( F_x^k \right)^k + \sum_{\Delta X} \left( \frac{\partial F_x}{\partial X} \right)^k \Delta X = 0 \]  

(23)

The solution procedure amounts to solve the blocked matrix according to the algorithm shown in Eq. (23), where \( X \) stands for oil pressure, mass fractions of oil and water.

**Results**

Before to solve 2D and 3D flows whose solutions can be compared with results available in the literature, the model was exhaustively tested with problems specially conceived for checking the correctness of the algorithm, characteristics of the solution, like symmetry, and code implementation. Following, comparisons were made with classical problems described in the literature.

**Two-phase Flow in a Five-Spot Geometry.** The piston-type flow (water and oil) of Yanosick and McCracken[14] with the data shown in Table 1 and the following expressions for the permeabilities, as suggested by Palagi [11],

\[ k_w^* = S_w^2 \]  

(24)

\[ k_o^* = (1 - S_w^2)^2 = S_o^{*2} \]  

(25)

were solved using the grid shown in Fig. 3 with 20x20 control volumes and a Cartesian grid with the same number of volumes. The oil recovered plot is shown in Fig. 4, where one can see the good agreement between the results of the present work with the curvilinear grid and the ones obtained by Palagi[11]. As a second test problem, two-phase flow in a 5-spot geometry, as described in Marcondes [12] was solved. Table II and III presents the data used and Fig. 5 presents the comparison. In this problem Marcondes [12] used two different types of Voronoi grids, not shown here, while in this work the same curvilinear grid shown in Fig. 3 was employed. Again one can see good agreement between the
results.

Three-Dimensional Two-Phase Flow. Fig. 6 shows a 19x10x5 curvilinear grid used for the solution of the two-phase flow in a petroleum reservoir with two injections and six production wells and a geological fault identified by the dark line. This problem was solved and compared with the results of Marcondes [12] where hexagonal and hybrid (hexagonal-radial) grids of Voronoi type were used. A detailed comparison was made were oil recovered and pressure at the wells were checked. The reservoir data and flow rates used can be found in [12]. For illustration purposes only, the right part of Fig. 6 shows the 0.4 and 0.6 isolevels of water saturation.

Three-Dimensional “Three Phase Flow”. In this pseudo three-phase flow the densities and viscosities of the phases were made equal and the permeabilities of the oil, gas and water phases are equal to their respective saturations, that is

\[ k^{io} = S^{io} \]  \hspace{1cm} (26)
\[ k^{ro} = S^{io} \]  \hspace{1cm} (27)
\[ k^{go} = S^{io} \]  \hspace{1cm} (28)

The geometry under consideration is a deformed cube, in order to create a non-orthogonal grid, which resembles a 3D five-spot, as shown in Fig. 7. Since the main goal is only to check the mass conservation constraint, the initial saturation of water for oil and 0.5 for oil and gas were used. Fig 8 shows the saturation of the water, oil and gas, after 0.3 VPI, along the line formed joining the center of the volumes shown in Fig. 7.

Modified SPE01 test problem. This final problem aims to test the methodology in a situation where the gas phase appearance/disappearance happens. To reach this goal the problem used the full data of the SPE01 test problem with the exception that an arial situation is considered. A 5x5 Cartesian grid is employed with a well in the central control volume. The simulation is performed along 8005 days and in the beginning of the simulation the water and oil saturation is 0.0001 and 0.999, respectively. The well produces oil for 1205 days, and due to the pressure decrease the gas phase appears. Following the simulation, the well is closed for some time and then water begins to be injected. This increases the reservoir pressure and makes the gas phase to disappear. This simulation was compared with the SIMPAR code [13] and the results are in good agreement, as can be seen in Fig. 9.

Algorithm implementation. The algorithm was implemented in C++ Object Oriented Programming with a powerful graphical user interface integrated with 3D visualization tools. The resulting software is extremely user-friendly and offers 3D visualization of the results any time of the simulation.

Conclusions
The results obtained with the numerical model implemented in this work encourages the use of the mass fractions as dependent variables. The numerical model developed is capable of handling irregular reservoirs by using boundary-fitted grids, and it is also suitable for petroleum reservoir simulations where grids following geological structures are required.

Nomenclature

\[ \phi \] = porosity
\[ \rho^o \] = mean density
\[ \lambda \] = phase mobility
\[ \Phi \] = phase potential
\[ m^w, m^o, m^g \] = mass flow rate of water, oil and gas
\[ \chi_i \] = mass fraction of the i component
\[ \chi^{io} \] = ratio of oil mass in oil phase by mass of oil phase
\[ p^o \] = oil pressure
\[ p^{ow} \] = oil-water capillarity pressure
\[ p^{og} \] = oil-gas capillarity pressure
\[ J \] = jacobian of the coordinate transformation
\[ \xi, \eta, \gamma \] = curvilinear coordinate system
\[ F \] = fault coefficients
\[ k^{io}, k^{ro}, k^{go} \] = relative permeability
\[ S^o \] = saturation

References

**TABLE 1-PISTON TYPE FLOW**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
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<tbody>
<tr>
<td>Length</td>
<td>402.33 m (1320 ft)</td>
</tr>
<tr>
<td>Width</td>
<td>402.33 m (1320 ft)</td>
</tr>
<tr>
<td>Depth</td>
<td>6.09 m (20 ft)</td>
</tr>
<tr>
<td>Porosity</td>
<td>φ = 0.08</td>
</tr>
<tr>
<td>Absolute Permeability</td>
<td>k = 0.0125 μm² (12.5 mD)</td>
</tr>
<tr>
<td>Initial Pressure</td>
<td>Pᵢ = 689.4 kPa (100 psi)</td>
</tr>
<tr>
<td>Initial Saturation</td>
<td>Sᵢ = 0</td>
</tr>
<tr>
<td>Prod. and Inj. Flow Rate</td>
<td>q = 9.534 m³/day (60 STB/day)</td>
</tr>
<tr>
<td>Density</td>
<td>ρᵢ = 1000 kg/m³</td>
</tr>
<tr>
<td>Formation Volume Factor</td>
<td>Bᵢ = Bₚ = 1 at 689.4 kPa (100 psi)</td>
</tr>
<tr>
<td>Compressibility</td>
<td>cᵢ = cₚ = 1.45033x10⁻⁸ Pa⁻¹ (1.0x10⁻⁵ psi⁻¹)</td>
</tr>
<tr>
<td>Water Viscosity</td>
<td>μᵢ = 1 mPa.s (1 M cp)</td>
</tr>
<tr>
<td>Oil Viscosity</td>
<td>μₚ = 1.0 mPa.s (1.0 cp)</td>
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</table>

**TABLE 2-THREE DIMENSIONAL TWO PHASE FLOW**

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<tr>
<td>Depth</td>
<td>h = 15 m (49.2126 ft)</td>
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<tr>
<td>Well Radius</td>
<td>rᵢ = 0.12192 m (0.4 ft)</td>
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<tr>
<td>Porosity</td>
<td>φ = 0.3</td>
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<tr>
<td>Absolute Permeability</td>
<td>k = 0.3 μm² (300 mD)</td>
</tr>
<tr>
<td>Initial Pressure</td>
<td>Pᵢ = 20685 kPa (3000 psi)</td>
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<tr>
<td>Initial Saturation</td>
<td>Sᵢ = 0.20</td>
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<tr>
<td>Prod. and Inj. Flow Rate</td>
<td>q = 2.76x10⁻⁹ m³/s (1500 STB/day)</td>
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<td>Density</td>
<td>ρᵢ = 1000 kg/m³</td>
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<tr>
<td>Formation Volume Factor</td>
<td>Bᵢ = Bₚ = 1 at 20685 kPa (3000 psi)</td>
</tr>
<tr>
<td>Compressibility</td>
<td>cᵢ = cₚ = 7.25163x10⁻⁹ Pa⁻¹ (5.0x10⁻⁵ psi⁻¹)</td>
</tr>
<tr>
<td>Water Viscosity</td>
<td>μᵢ = 10⁻⁵[1 + 1.45x10⁻¹²(P - 1.38x10⁷)] Pa.s</td>
</tr>
<tr>
<td>Oil Viscosity</td>
<td>μₚ = 1.163x10⁻⁵[1 + 1.45x10⁻¹²(P - 1.38x10⁷)] Pa.s</td>
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TABLE 3-RELATIVE PERMEABILITY FOR THE 5-SPOT PROBLEM

<table>
<thead>
<tr>
<th>$S^w$</th>
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<th>$K^{w}$</th>
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<td>0.22</td>
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<td>0.00</td>
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<td>0.0000</td>
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<td>0.0000</td>
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<td>1.00</td>
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<td>1.00</td>
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Fig. 1-Elemental control volume - Physical and computational domain

Fig. 2-Control volume and its neighbors for deriving the equivalent wellblock radius

Fig. 3-Grid used for the piston-type flow in a Five-Spot geometry
Fig. 4-Oil recovered versus PVI for the Piston-type flow in a Five-Spot geometry. Comparison with Palagi[11]

Fig. 5-Oil recovered versus PVI for the two-phase flow in a Five-Spot geometry. Comparison with Marcondes et al [12]

Fig. 6-Grid employed (19x10x5) and saturation fields for a 3D two-phase flow
Fig. 7 - Tridimensional three-phase flow simulation. Grid employed

Fig. 8 - Saturation after 0.3 VPI along the line shown in Fig. 7

Fig. 9 - Gas saturation in the cell containing the well
Fig. 10 - Reservoir average pressure in the cell containing the well

Fig. 11 - Oil saturation in the cell containing the well