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SEQUENTIAL IMPLICIT APPROACH FOR COMPOSITIONAL RESERVOIR SIMULATION IN CONJUNCTION WITH UNSTRUCTURED GRIDS

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Abstract. *Various formulations are used to solve numerically complex systems of partial differential equations that describe important physical phenomena. The approach for solving the resulting equations from the modeling of the fluid flow has a great effect on the simulator's performance making its use possibly prohibitive in practice from computational point of view. In compositional reservoir simulation, the numerical formulations are usually divided into two broad classes: volume balance and mass balance. The former formulation uses a volume balance equation to determine the pressure for each gridblock. In this work, a semi-implicit volume balance formulation was implemented into The University of Texas Compositional Simulator (UTCOMP) for unstructured grids in conjunction with the finite-volume method. The semi-implicit formulation implemented is implicit in pressure and phase saturations and explicit in moles (IMPSAT). This formulation is compared with the original IMPEC (implicit pressure, explicit compositions) formulation of UTCOMP, which was previously validated with analytical solutions and commercial simulators, implemented to unstructured grids. The results obtained suggest that for coarse grids, the IMPES formulation presents the lowest computational time, however as the grids are refined the semi-implicit approach improves its performance in terms of computational time when compared to the IMPES formulation.*

Keywords: *Compositional reservoir simulation, Segregated formulation, IMPEC, IMPSAT, Finite-volume method.*

1. INTRODUCTION

Several numerical formulations have been developed for solving the governing partial differential equations arising from modeling fluid flow for compositional simulations in porous media. In general, these formulations are classified as Implicit Pressure Explicit Composition (IMPEC), Implicit Pressure and Saturation (IMPSAT), or Fully Implicit Method (FIM). From these classes the formulation with the lowest implicitness degree is the IMPEC, while the FIM class has the highest implicitness degree. A high implicitness degree reflects in the possibility of larger time-step sizes while increase the computational cost per time-step, due to increasing in the unknowns to be solved from the discretized equations, and hence larger linear system of equations. IMPSAT formulations are between IMPEC and FIM in both aspects as it allows for larger time-steps than IMPEC formulations with computational cost per time-step smaller than FIM formulations.

Several procedures for solving pressure and saturation implicitly (IMPSAT) have been proposed in the literature (Branco and Rodrigues, 1996; Kendall et al., 1983; Spillette et al., 1973). However, the IMPSAT approach proposed by Watts (1986) and adopted in this work has similar features as the original IMPEC formulation of the UTCOMP simulator. The great advantage of such approach compared to other IMPSAT approaches is just one flash calculation per time-step and the decoupling of pressure and saturations equations which allow for the solution of a smaller linear systems of equations. More details regarding Watts' original formulation can be found in the literature (Quandalle and Savary, 1992; Cao, 2002; Haukas, 2006; Fernandes, 2014; Fernandes et al. 2014). IMPSAT formulations became famous due to the strong non-linear behavior of the relative permeability and capillary pressure with respect to saturation. Fernandes (2014) and Fernandes et al. (2014) extended the Watts' original formulation from three-phase flow to a four phases flow using Cartesian grids.

Another important aspect in reservoir simulation is the gridding technique. Reservoirs can present complex geometries and also associated, in general, with complex features such as geological faults, fractures, and deviated wells. The geometry and features of a reservoir can be better exploited by using unstructured grids that not only allow

for the better mapping of such geometries but also for better local grid refinement. The first use of unstructured grids in reservoir simulation was performed by Heinemann and Brand (1988) in conjunction with PEBI grids (Perpendicular Bisector). The first use of the Element based Finite Volume Method (EbFVM), originally named as Control Volume Finite Element Method (CVFEM), in reservoir simulation was performed by Rozon (1989); he used it to solve a single-phase flow using quadrilateral elements. Cordazzo (2006) solved the two-phase flow (water and oil) in conjunction with the EbFVM using triangular and quadrilateral elements. Marcondes and Sepehrnoori (2010) used the EbFVM for the fully implicit, fully coupled, isothermal compositional simulation in conjunction with triangular and quadrilateral elements. Recently, Marcondes et al. (2013) and Santos et al. (2013) implemented the EbFVM for 3D isothermal compositional reservoir simulation. Also, using the EbFVM approach, Fernandes et al. (2013) has investigated the use of several interpolation functions in conjunction with 2D compositional reservoir simulation. More recently, Fernandes et al. (2014) extended the Total Variation Diminishing scheme (TVD) implemented by Fernandes et al. (2013) to the 3D EbFVM considering the hexahedron element.

In this work, an IMPSAT formulation proposed by Watts (1986) was implemented into the UTCOMP simulator for unstructured grids using the EbFVM, a powerful technique that not only allows for the discretization of arbitrary geometries, such as very complex reservoirs, but also for the increasing in the spatial discretization accuracy and reduction of grid orientation effects. UTCOMP was developed at The Center for Petroleum and Geosystems Engineering at The University of Texas at Austin for the simulation of enhanced recovery processes. The UTCOMP simulator is a multiphase/multi-component compositional equation-of-state simulator, which can handle the simulation of several enhanced oil recovery processes. The original numerical procedure of the UTCOMP simulator is an IMPEC formulation based on Àcs et al. (1985) for Cartesian grids and was extended to 2D unstructured grids by Fernandes et al. (2012) and to 3D unstructured grids by Araújo et al. (2015).

2. MATHEMATICAL MODEL

The Watts' formulation is basically an adaptation of the method of Spillette et al. (1973) combined with the formulation of Ács et al. (1985), where the volume error constraint is added to pressure and saturation equations in order to use just only one flash calculation per time-step. In this section, we show the molar balance equations, the pressure equation, and the new saturation equations that are included into the original formulation of Ács et al. (1985).

If the advection is the only transport mechanism involved, the molar balance equations according to Chang (1990) are given by

$$\frac{1}{V_b}\frac{\partial N_k}{\partial t} = \sum_{j=1}^{N_p} \vec{\nabla}\cdot\left(x_{kj}\xi_j \frac{k_{rj}}{\mu_j} \bar{\bar{K}}\cdot\vec{\nabla}\Phi_j \right) - \frac{q_k}{V_b}, \qquad k = 1,\ ...,\ N_c,\ N_c+1, \tag{1}$$

where N_k is the moles of component k, V_b is the bulk volume, x_{kj} is the mole fraction of component k in phase j, ξ_j is the molar density, respectively, q_k is the molar rate of component k through the well, N_c is the number of hydrocarbon components, N_c+1 denotes the water component, N_p is the number of phases, k_{rj} and μ_j are the relative permeability and viscosity of phase j, respectively, $\bar{\bar{K}}$ is the absolute permeability tensor, and Φ_j is the hydraulic potential of phase j which is defined by

$$\Phi_j = P - \rho_j g D - P_{cjr}, \tag{2}$$

where P is the pressure of oil phase, ρ_j is the mass density of phase j, g is the gravity, D is the depth which is positive in downward direction, and P_{crj} is the capillary pressure between phases j and r.

Fluid phase equilibrium between the hydrocarbon phases is considered (water is not considered in any flash calculation, in this work). This assumption considers that the chemical potential of all phases are the same. This can be expressed in terms of the equality of the fugacities (f) of the phases, which can be stated as follows:

$$f_i^2 - f_i^l = 0, \qquad i = 1,\ ...,\ N_c, \quad l = 3, N_p, \tag{3}$$

where f_i^2 is the fugacity of the *i-th* component in phase *2*, f_i^2 is the fugacity of the *i-th* component in phase l, 2 denotes the oleic phase, *3* denotes the gas phase, and *4* denotes the second hydrocarbon liquid phase.

Fugacity and PVT properties are evaluated using the Peng-Robinson Equation of State (EOS) (Peng and Robinson, 1978). The flash procedure used considers a fixed and known pressure, temperature, and global compositions (isothermal flash) in order to evaluate the phase compositions and fluid properties. Further details of this procedure and the phase stability procedures can be found in Perschke (1988) and Chang (1990).

The pressure equation is obtained from the equality between the formation pore volume (V_p) and the total fluid volume (V_t), which can be written as

$$\phi_0 c_f \frac{\partial P}{\partial t} = \frac{1}{V_b}\left(\frac{\partial V_t}{\partial P}\right)_N \frac{\partial P}{\partial t} + \sum_{k=1}^{N_c+1}\left(\frac{\partial V_t}{\partial N_k}\right)_{P,N_s(s\neq i)} \left[\sum_{j=1}^{N_p} \vec{\nabla}\cdot\left(x_{kj}\xi_j \frac{k_{rj}}{\mu_j} \bar{\bar{K}}\cdot\vec{\nabla}\Phi_j \right) + \frac{q_k}{V_b} \right], \tag{4}$$

where ϕ_0 is the porosity at a reference pressure, c_f is the rock compressibility, and t is the time.

The saturation equation is also a volume balance for a given phase, and is written in terms of velocity, since it is more appropriate for decoupling procedure that will be further explained (Watts, 1986).

$$\frac{1}{V_b}\frac{\partial}{\partial t}\left(S_\ell V_p\right)=\frac{1}{V_b}\left(\frac{\partial V_\ell}{\partial P}\right)_N\frac{\partial P}{\partial t}+\sum_{k=1}^{N_c+1}\left(\frac{\partial V_\ell}{\partial N_k}\right)_{P,N_s(s\neq i)}\left(\sum_{j=1}^{N_p}\vec{\nabla}\cdot\left(x_{kj}\xi_j\vec{v}_j\right)+\frac{q_k}{V_b}\right),\qquad \ell=1,...,N_p, \tag{5}$$

where S_ℓ is the saturation of the ℓ-*th* phase, V_p is the pore volume, V_ℓ is the volume of the ℓ-*th* phase, $\vec{v}_j$ is the velocity of the *j-th* phase

Analysis of Eq. (5) shows that summing up these equations over all phases will result in Eq. (4).

As suggested by Watts (1986) the phase velocity that is needed in Eq. (5) is evaluated from the total velocity rather than simply substituting Darcy's law. The equations for the phase velocity for a full tensor permeability can be obtained using the procedure of Kaasschieter (1999) for two phase flow, which was extended by Fernandes (2014) for three and four hydrocarbon phases. Fernandes (2014) also extended this to the volumetric flow that will be important in this text. The phase velocity is written as

$$\vec{v}_j=f_j\left[\vec{v}_t+\sum_{m=1}^{Np}\frac{k_{rm}}{\mu_m}\overline{\overline{K}}\cdot\left(g\left(\rho_j-\rho_m\right)\vec{\nabla}D+\vec{\nabla}\left(P_{cjo}-P_{cmo}\right)\right)\right], \tag{6}$$

where

$$\vec{v}_t=\sum_{i=1}^{Np}\vec{v}_i=-\sum_{j=1}^{Np}\frac{k_{rj}}{\mu_j}\overline{\overline{K}}\cdot(\vec{\nabla}P+\vec{\nabla}P_{cjo}-g\rho_j\vec{\nabla}D), \tag{7}$$

and

$$f_j=\frac{k_{rj}/\mu_j}{\sum_{m=1}^{Np}k_{rm}/\mu_m}, \tag{8}$$

where, $\vec{v}_t$ is the total fluid velocity , and f_j is called the fractional flow, which is defined above.

Substituting Eq. (6) into (5) yields

$$\begin{aligned}\frac{1}{V_b}\frac{\partial}{\partial t}\left(S_\ell V_p\right)=&\frac{1}{V_b}\left(\frac{\partial V_\ell}{\partial P}\right)_N\frac{\partial P}{\partial t}+\sum_{k=1}^{N_c+1}\left(\frac{\partial V_\ell}{\partial N_k}\right)_{P,N_s(s\neq i)}\left(\frac{q_k}{V_b}\right)+\\ &\sum_{k=1}^{N_c+1}\left(\frac{\partial V_\ell}{\partial N_k}\right)_{P,N_s(s\neq i)}\left(\sum_{j=1}^{N_p}\vec{\nabla}\cdot\left[x_{kj}\xi_j f_j\left(\vec{v}_t+\sum_{m=1}^{Np}\frac{k_{rm}}{\mu_m}\overline{\overline{K}}\cdot\left(g\left(\rho_j-\rho_m\right)\vec{\nabla}D+\vec{\nabla}\left(P_{cjo}-P_{cmo}\right)\right)\right)\right]\right).\end{aligned} \tag{9}$$

Equation (9) is the final saturation equation in terms of total velocity. The next section is devoted to showing the numerical discretization applied to the above equation.

3. APPROXIMATED EQUATIONS

In the EbFVM the domain is divided into elements. The most common used elements are triangles and quadrilaterals for 2D grids, and hexahedrons, tetrahedrons, prisms, and pyramids for 3D grids. All of these elements are considered here. The first step is to integrate the conservation equations into the control-volume and time. In the EbFVM, control-volumes are constructed around the grid vertices and are formed by assembling pieces of the elements surrounding such vertices. This procedure is illustrated in Figure 1. The pieces of the elements that compose the control-volumes are called subcontrol-volumes (SCV) and are interconnected by interfaces called integration points (IP), which are the points where the advection and diffusion fluxes are to be computed. The good point of such approach is the all calculations are carried out inside the elements.

Integrating the pressure equation over time and an arbitrary control-volume around a node p connected to n_e elements, and applying the Green theorem to the advection terms yields

$$\left[\phi_{0,p}c_f V_{b,p}-\frac{\partial V_{t,p}^0}{\partial P}\right]\left(P_p-P_p^0\right)=\Delta t\sum_{k=1}^{N_c+1}\frac{\partial V_{t,p}^0}{\partial N_k}\left[\sum_{j=1}^{N_p}\sum_{l=1}^{n_{ip}}\left(x_{kj}^0\xi_j^0\frac{k_{rj}^0}{\mu_j^0}\overline{\overline{K}}\cdot\vec{\nabla}\left(P-\rho_j^0 gD-P_{cjr}^0\right)\right)_l\cdot\Delta\vec{A}_l+q_{k,p}^0\right]+\left(V_{t,p}^0-\phi_p^0V_{b,p}^0\right), \tag{10}$$

where the superscript 0 denotes an explicit variable, and the gradient operator is approximated using the shape functions for a given element as

$$\left.\frac{\partial P}{\partial x}\right|_l=\sum_{i=1}^{n_v}\frac{\partial N_i\left(\xi_l,\eta_l,\gamma_l\right)}{\partial x}P_i;\left.\frac{\partial P}{\partial y}\right|_l=\sum_{i=1}^{n_v}\frac{\partial N_i\left(\xi_l,\eta_l,\gamma_l\right)}{\partial y}P_i;\left.\frac{\partial P}{\partial z}\right|_l=\sum_{i=1}^{n_v}\frac{\partial N_i\left(\xi_l,\eta_l,\gamma_l\right)}{\partial z}P_i\,, \tag{11}$$

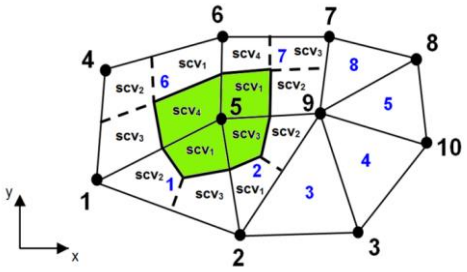

Figure 1. Illustration of a control-volume for the EbFVM approach.

where the n_v is the number of vertices of a given element, N_i's are the shape functions, ξ_l, η_l, and γ_l are the coordinates of the point l in the transformed plane, and P_i is the pressure evaluated at vertex i. Derivatives are computed in the same manner for any other variable. The derivatives of the shape functions with respect to the coordinates in the physical plane are shown in several other works such as in Maliska (2004), Marcondes and Sepehrnoori (2010), Fernandes et al. (2012), and Araújo et al. (2015).

Note that the pressure equation is solved considering the terms that are function of saturation, such as relative permeability and saturation, explicitly as it is done in an IMPEC formulation. According to Watts (1986), the next step is to compute the semi-implicit total velocities for each control-volume face. However, such approach is not convenient to unstructured grids since the control-volume faces are not align to the Cartesian axis, which would increase complexity and the number of mathematical operations needed. Therefore, the semi-implicit total flux for an integration point l is written as

$$F_t\big|_l = -\sum_{j=1}^{Np} \frac{k_{rj}^0}{\mu_j^0}\bigg|_l \bar{\bar{K}} \cdot (\vec{\nabla}P + \vec{\nabla}P_{cjo}^0 - g\rho_j^0\vec{\nabla}D)\Big|_l \cdot \Delta\vec{A}_l, \tag{12}$$

and Eq. (10) is approximated as

$$S_{\ell,p}V_{p,p} - S_{\ell,p}^0 V_{\ell,p}^0 = \frac{\partial V_{\ell,p}^0}{\partial P}\left(P_p - P_p^0\right) + \Delta t \sum_{k=1}^{N_c+1} \frac{\partial V_{\ell,p}^0}{\partial N_k} q_{k,p} + \Delta t \sum_{k=1}^{N_c+1} \frac{\partial V_{\ell,p}^0}{\partial N_k} \sum_{j=1}^{N_p} \sum_{l=1}^{n_{ip}} x_{kj,l}^0 \xi_{j,l}^0 F_{j,l}\ , \tag{13}$$

where,

$$F_{j,l} = \frac{k_{rj,l}\big/\mu_{j,l}^0}{\sum_{m=1}^{Np} k_{rm,l}\big/\mu_{m,l}^0}\left(F_{t,l} + \sum_{m=1}^{Np}\frac{k_{rm,l}}{\mu_{m,l}^0}\left(g\left(\rho_{j,l}^0 - \rho_{m,l}^0\right)\bar{\bar{K}}\cdot\vec{\nabla}D\cdot\Delta\vec{A}_l + \bar{\bar{K}}\cdot\vec{\nabla}\left(P_{cjo,l} - P_{cmo,l}\right)\cdot\Delta\vec{A}_l\right)\right). \tag{14}$$

The procedure used to solve Eq. (13) was the exact Newton's method. Note that as the saturations sum up to unity, it is only needed to solve N_p-*1* saturations for each grid vertex. Since one of the saturations becomes a dependent variable, it is need to be careful when computing the Jacobian matrix to make sure that this consideration is being taken into account. Phase disappearance is also considered in this step as phase is considered to disappear when its saturation goes below zero.

The next step is to evaluate the total number of moles of each component according to

$$N_{k,p} = N_{k,p}^0 + \Delta t q_{k,p} + \Delta t \sum_{j=1}^{N_p}\sum_{l=1}^{n_{ip}} x_{kj,l}^0 \xi_{j,l}^0 F_{j,l}\ , \tag{15}$$

where the phase volumetric flux at interface l, $F_{j,l}$, was computed iteratively along with the saturations.

The algorithm of this formulation is presented in the flowchart of Figure 2.

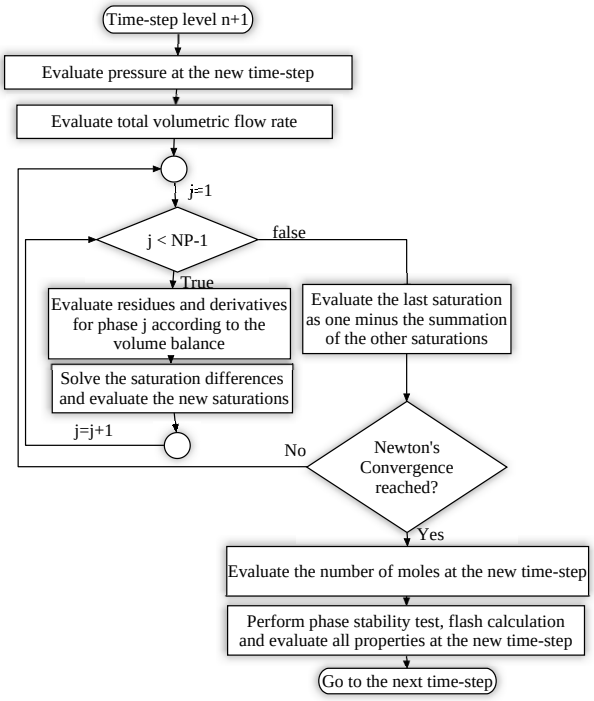

Figure 2. Watts' formulation flowchart.

4. RESULTS

In this section, the results of the IMPSAT formulation in conjunction with the EbFVM approach are tested and compared with the IMPEC formulation associated with the EbFVM implemented by Fernandes et al. (2012) and Araújo et al. (2013). Three case studies are presented. In the first case study, we compare the performance of the IMPSAT formulation implemented with the IMPEC formulation previously implemented in a 2D reservoir with CO_2 flooding, while in the second case the same reservoir is considered but now we also consider variation in z-direction.

For Case 1, two set of grids were considered. The first set considers only quadrilateral elements, while the second set considers only triangular elements. Each set contains three distinct grids that differ by number of vertices. The purpose here is to verify how the refinement affects each element type for both formulations. The reservoir data for Cases 1 and 2 is given in Table 1

Table 1. Reservoir data for Cases 1 and 2.

Property	Value
Length, width, and thickness	243.83 m, 243.83 m, and 60.96 m
Porosity	0.30
Initial water saturation	0.25
Initial pressure	20.65 MPa
Permeability in x, y, and z directions	1.97×10^{-13} m^2, 1.97×10^{-13} m^2, and 1.97×10^{-14} m^2
Formation temperature	299.82 K
Gas injection rate	5.66×105 m^3/d
Producer's bottom hole pressure	20.65 MPa
Fluid in-place composition (CO_2, C_1, nC_{16})	0.01, 0.19, 0.80
Injected Fluid Composition (CO_2, C_1, nC_{16})	0.95, 0.05, 0.00

Figure 3 presents the saturation field of the CO_2 rich phase, which was labeled as gas, at 500 days of simulation obtained with the finest grids used in this study. From this figure, it is possible to see a good agreement of the saturation field between both formulations for quadrilaterals (Figure 3a and 3b), and also for triangular grids (Figures 3c and 3d).

For this case, the time-step was observed to be almost constant during most part of the simulation and equals to the maximum time-step allowed. These maximum time-steps are shown in Table 2 for the finest grids. It can be observe that the maximum time-step obtained for the IMPSAT is more than two times larger than that of IMPEC. The time-steps are controlled by changes in some properties according to the procedure given by Chang (1990). The parameters

used to control the time-step were adjusted empirically in this work, in order to find the optimum time-step profile that do not produce spurious oscillations.

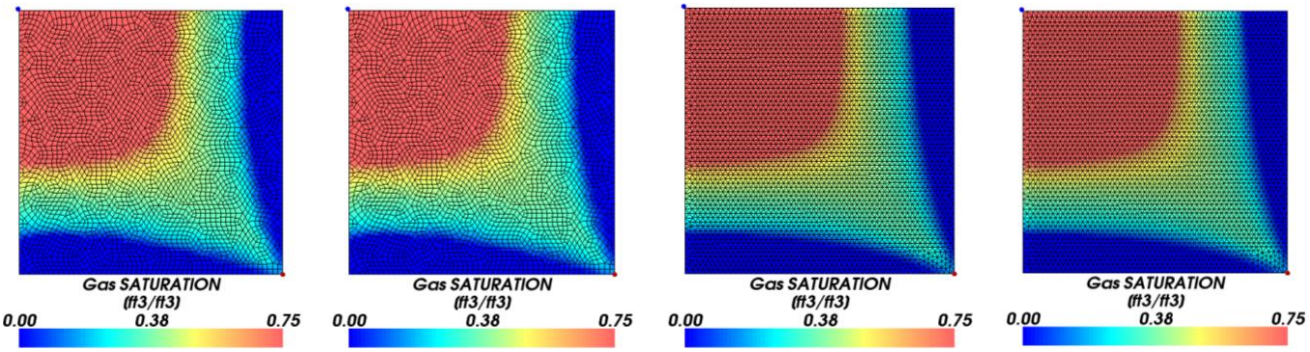

Figure 3. CO_2 rich phase at 500 days of simulation. a) IMPEC and b) IMPSAT, 3,387 vertices grid with 3,282 quadrilateral elements; c) IMPEC and d) IMPSAT, 3329 vertices grid with 6444 triangle elements

Table 2. Maximum time-step (days) for Case 1.

Formulation	3387 vertices quadrilateral elements grid	3329 vertices triangle elements grid
IMPEC	0.035	0.025
IMPSAT	0.100	0.060

The overall CPU times obtained for all simulations are presented in Tables 3 and 4, where it can be seen that the IMPSAT formulation performed better for all grids tested.

Table 3. CPU time (s) of all simulations - Case 1 using 2D unstructured grids of quadrilateral elements.

Formulation	1199 vertices	2661 vertices	3387 vertices
IMPEC	95.23	564.32	824.13
IMPSAT	61.74	341.75	519.24

Table 4. CPU time (s) of all simulations - Case 1 using 2D unstructured grids of triangular elements.

Formulation	1,220 vertices	2,330 vertices	3,329 vertices
IMPEC	99.31	544.25	1,134.59
IMPSAT	91.25	397.33	864.75

We now present the results for Case 2. The results will be present in a similar way to that of the previous Case. Although the 3D EbFVM UTCOMP had been tested to hexahedron, tetrahedron, prism and pyramid elements, only the results for hexahedron will be presented here. Results for the other elements can be found in Fernandes (2014).

The CO_2 rich phase saturation profile is shown at 500 days for the finest hexahedron grid in Figure 4. From this figure, it can be observed a good agreement of the saturation profiles between both formulations.

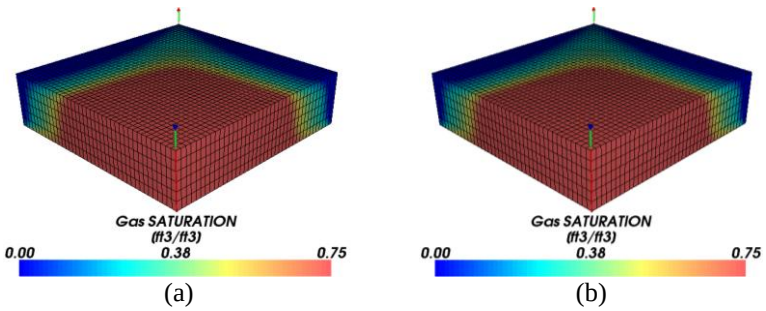

Figure 4. CO_2 rich phase at 500 days of simulation for the hexahedron grid with 11,767 vertices. a) IMPEC and b) IMPSAT.

The maximum time-steps obtained for the grid with 11,767 vertices grid are presented in Table 5. Again, from this table it can be observed that IMPSAT allowed an increased of the maximum time-step by a factor of about three times.

Table 5. Maximum time-step (days) for Case 2.

Formulation	1,024 vertices	6,480 vertices	11,767 vertices
IMPEC	0.35	0.07	0.05
IMPSAT	1.00	0.20	0.20

However, from Table 6 it can be observed that even with the increasing in the time-step, the IMPSAT formulation CPU times were comparable to those obtained using the IMPEC formulation when 3D grids are used.

Table 6. CPU time (s) of all simulations for Case 2.

Formulation	1,024 vertices	6,480 vertices	11,767 vertices
IMPEC	34.99	1,173.29	3,162.33
IMPSAT	36.40	1,204.63	2,810.85

5. CONCLUSIONS

In this work, the sequential IMPSAT formulation of Watts was successfully adapted and implemented for unstructured grids using the EbFVM approach. The IMPSAT formulations was shown to achieve larger time-steps than the IMPEC for not more than three times.

The IMPSAT formulation was shown to present better CPU times than those obtained using the IMPEC formulation for 2D grids, but comparable CPU times for 3D grids, although the IMPSAT's performance increased as the grid was refined. It shows that combining both formulations in one framework may lead to more efficient computational time for the simulations.

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