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SPECIFIED ADAPTIVE IMPLICIT METHOD FOR UNSTRUCTURED GRIDS IN COMPOSITIONAL RESERVOIR SIMULATION

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Abstract. *Compositional reservoir simulation is an important tool for predicting oil and gas production and it has been largely used in the last decades. Since compositional reservoir simulation, in general, involves solution of a large number of coupled partial differential equations representing the physical system, the numerical implementation of such model is a complex step. Different numerical approaches have been proposed in literature to optimize the CPU time of the numerical formulations. These formulations present many similarities; therefore, they are organized in major groups, which share some basic features. Two of these groups are of interest in this work: IMPEC (Implicit Pressure/Explicit Composition) and FI (Fully Implicit). In the IMPEC formulation, the pressure is evaluated implicitly, and the remaining variables explicitly. Fully Implicit (FI) methods, in the other hand, compute all the primary variables implicitly. Both techniques present advantages and disadvantages. In this work, a new formulation is proposed that combine features of both IMPEC and FI approaches. We call the new formulation the Specified Adaptive Implicit Method (SAIM), since the grid blocks that are treated as FI are fixed during the whole simulation. Herein the well grid blocks are always treated as FI; the neighbors of these grid blocks can also be treated as FI, and also the neighbors of the last set of grid blocks that were treated as FI can also be treated as fully implicit as well. The performance of SAIM is compared with the FI and IMPEC approaches in terms of average time step and total CPU time required for each simulation. The results obtained indicate the SAIM formulation is able to outperform the IMPEC in many situations.*

Keywords: *SAIM, IMPEC, FI, Compositional Reservoir Simulation, EbFVM*

1. INTRODUCTION

Oil production involves a series of time and economic demanding steps; hence, it depends greatly on accurate data and optimal processes. Reservoir simulation is a complex tasks in the oil and gas production. Fluid properties, phase stability, well effects, all together in a single package, require large computational effort at each computational time level. Acquiring valuable data to predict field behavior is key task in this process. Accuracy alone, however, is not the goal of commercial and academic simulators. Computational time is also an important issue to be considered. Hence, works on optimal simulation performance are vastly found in the literature (Fernandes, 2014; Watts, 1986; Varavei et al, 2013).

The work presented here is based on the UTCOMP (Chang, 1990), a compositional simulator first implemented with an IMPEC (Implicit Pressure/ Explicit Composition) formulation based on Ács et al. (1985), developed at The Center for Petroleum and Geosystems Engineering at The University of Texas at Austin. The UTCOMP is a multiphase/multi-component compositional equation-of-state simulator, capable of handling various enhanced oil recovery processes. As the name suggests, only the pressure is computed implicitly here, while all remaining properties are calculated explicitly. This approach has two main advantages. First, the linear system solved is the small, since there is only a single unknown per grid block. Second, no iterations are performed within a time step. Both features produce an inexpensive numerical approach per time level. However, due to numerical stability issues, the IMPEC formulation cannot work with large time steps, especially in regions of large gradients or rates as for instance close to wells or

saturation fronts. In order to increase the implicitness of the IMPEC approach, we suggest that the wells and neighbors of the wells gridblocks to be evaluated using a fully implicit approach and the rest of the reservoir by an IMPEC approach. The formulation proposed here combines the original method implemented into UTCOMP with the work developed by Fernandes (2014), which added two fully implicit formulations to the UTCOMP simulator. Among them, a Fully Implicit (FI) formulation modified from Ács et al. (1985). FI methods are, in general, more stable and able to handle much larger time steps compared to the ones used by IMPEC approach. On the other hand, since not only the pressure is solved implicitly the computational work per time step increases. The total number of moles of each component is also computed in the Jacobian matrix, which increases the Jacobian size compared to the IMPEC approach. Another drawback using FI approach is the Newton iterations required in each time step, to resolve the non-linearities involved in the discretized equations.

Both (IMPEC and FI) techniques can be put together into a Specified Adaptive Implicit Method (SAIM). This is achieved by splitting the domain between FI and IMPEC volumes. The gridblocks associated with the wells (defined as those grid blocks connected directly to the wells or neighbors of these grid blocks) will be evaluated using a fully implicit formulation and the remaining grid blocks are evaluated through an IMPEC formulation. This procedure allows stable runs with large time steps combined with much smaller Jacobian matrixes when compared to those used by FI methods. Ultimately, the goal is to improve the performance of the UTCOMP simulator in comparison with the original simulator based on an IMPEC approach. This approach is implemented in conjunction the EbFVM (Element-based Finite Volume Method), using two-dimensional unstructured grids (Maliska & Hurtado, 2005; Marcondes & Seperhnoori, 2010). The results are presented in terms of oil and gas production curves, as well as time step sizes, and CPU times.

2. PHYSICAL MODEL

Evaluating an isothermal multiphase/multicomponent fluid flow in a porous media requires three sets of equations (Wang et al, 1997). These expressions are the material balances for each component, the phase equilibrium relations, and the constraint equations for the phase saturations and composition. The saturation restriction yields the pressure equation. Further development on this matter can be found in Chang (1990). The equations to evaluate the pressure and number of moles as developed by Ács et al. (1985), can be respectively, written as

$$\left[\phi^0 C_f - \frac{1}{V_b}\frac{\partial V_T^n}{\partial P}\right]\left(P^{n+1}-P^n\right) = \frac{\left(V_T^n - V_p^n\right)}{V_b} + \Delta t\sum_{k=1}^{n_c}\bar{V}_{Tk}^n\left\{\sum_{j=2}^{n_p}\vec{\nabla}\cdot\left(x_{kj}^n\xi_j^n\frac{k_{rj}^n}{\mu_j^n}\bar{\bar{K}}\cdot\vec{\nabla}\left(P^{n+1}+P_{cjr}^n-\rho_j^n gD\right)\right)-\frac{\dot{q}_k^n}{V_b}\right\}$$
$$+\Delta t\bar{V}_{Tw}^n\left\{\vec{\nabla}\cdot\left(\xi_w^n\frac{k_{rw}^n}{\mu_w^n}\bar{\bar{K}}\cdot\vec{\nabla}\left(P^{n+1}+P_{cwr}^n-\rho_w^n gD\right)\right)-\frac{\dot{q}_w^n}{V_b}\right\} \quad (1)$$

$$\frac{\left(N_k^{n+1}-V_k^n\right)}{V_b} = \Delta t\left\{\sum_{j=2}^{n_p}\vec{\nabla}\cdot\left(x_{kj}^n\xi_j^n\frac{k_{rj}^n}{\mu_j^n}\bar{\bar{K}}\cdot\vec{\nabla}\left(P^{n+1}+P_{cjr}^n-\rho_j^n gD\right)\right)-\frac{\dot{q}_k^n}{V_b}\right\} k=1,...,n_c \quad (2)$$

In the above equations, P is the volume pressure, Nk represents the total moles of a component k, Cf denotes the rock compressibility, $\phi 0$ is the standard porosity, and Vt, Vp, and Vb denote the total, porous and bulk volumes, respectively, xij is the mole fraction of the k component in the j phase, ξj is the phase molar density, μj denotes the phase viscosity and krj is the relative permeability of phase j, K is the absolute permeability tensor, ρj is mass density of phase j, g stands for the gravity, D is the depth which is positive in downward direction, n and n+1 denotes the previous and present levels, respectively. Fernandes (2014) modified these equations for a FI approach. In this work, we further modify Eqs. (1) and (2) to added together the FI formulation proposed by Fernandes (2014) and IMPEC approach of Ács et al. (1985), into the SAIM framework.

$$RP = \left[\phi^0 C_f - \frac{1}{V_b}\frac{\partial V_T^n}{\partial P}\right]\left(P^{n+1}-P^n\right) - \frac{\left(V_T^n - V_p^n\right)}{V_b} - \Delta t\sum_{k=1}^{n_c}\bar{V}_{Tk}^n\left\{\sum_{j=2}^{n_p}\vec{\nabla}\cdot\left(x_{kj}^m\xi_j^m\frac{k_{rj}^m}{\mu_j^m}\bar{\bar{K}}\cdot\vec{\nabla}\left(P^{n+1}+P_{cjr}^m-\rho_j^m gD\right)\right)-\frac{\dot{q}_k^m}{V_b}\right\}$$
$$-\Delta t\bar{V}_{Tw}^n\left\{\vec{\nabla}\cdot\left(\xi_w^n\frac{k_{rw}^m}{\mu_w^m}\bar{\bar{K}}\cdot\vec{\nabla}\left(P^{n+1}+P_{cwr}^m-\rho_w^m gD\right)\right)-\frac{\dot{q}_w^m}{V_b}\right\} \quad (3)$$

$$RN_k = \frac{\left(N_k^{n+1}-V_k^n\right)}{V_b} - \Delta t\left\{\sum_{j=2}^{n_p}\vec{\nabla}\cdot\left(x_{kj}^m\xi_j^m\frac{k_{rj}^m}{\mu_j^m}\bar{\bar{K}}\cdot\vec{\nabla}\left(P^{n+1}+P_{cjr}^m-\rho_j^m gD\right)\right)-\frac{\dot{q}_k^m}{V_b}\right\}, k=1,...,n_c \quad (4)$$

Two aspects should be highlighted for Eqs. (3) and (4). First, both equations are written in the residual form. The presence of implicit blocks makes Eqs. (1) and (2) to be a non-linear system, which demands a similar evaluation as a

FI formulation. Also, another issue that needs consideration is the evaluation of various terms at different time levels. The properties are computed either at the current time step (*n+1*), or the previous one (*n*). However, there is also the '*m'* time step level, which simply implies a property can be computed at both levels, depending on whether a given term is evaluated as IMPEC or FI, yielding different forms for Eqs. (3) and (4). Once the time level is defined, the Jacobian matrix of the pressure and mole residual equations is assembled. However, as explained earlier, only the pressure is computed implicitly for the IMPEC approach. Hence, the mole equations for the IMPEC blocks are removed from the linear system. Once the implicit variables are updated, the explicit moles are computed, the phase behavior is evaluated and the simulation proceeds on calculation of the other properties. As mentioned before, each time-step requires a Newton iterative procedure. Only after the convergence criteria is satisfied, the simulation advances for the next time level.

A two-dimensional EbFVM grid with nine vertices, with wells located at the first and last volumes, is used as an example to assemble the linear system. The wells blocks are evaluated using FI approach, while the remaining volumes are computed as IMPEC. We now consider a two-component fluid case, as a simple case study. The full matrix takes the form shown in Fig. 1.

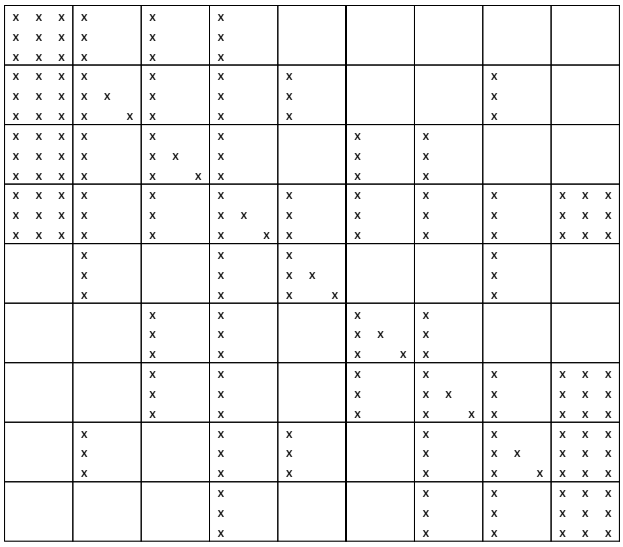


Figure 1. Full Jacobian matrix

The wells or wells' neighbors are always evaluated implicitly, with range varying according to user's choice. The reason behind this choice are the high phase velocities present in the region around the well, which are responsible for most of the IMPEC instabilities. By setting this region as FI, it is possible to increase the simulation time step and still produce accurate results. At the same time, by only using few implicit blocks, the Jacobian matrix size is similar to the one from IMPEC approach. The size of the linear system given in Fig. 1 can be reduced by removing the already mentioned explicit equations. Figure 2 shows the final matrix.

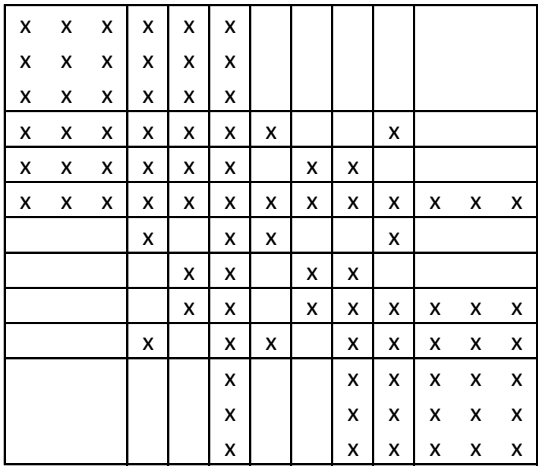


Figure 2. Reduced Jacobian matrix

It is possible to see that the size of the Jacobian matrix grows as the number of implicit blocks increases. At the same time, more FI gridblocks means more stable runs. The implicitness level can be set in three different ways, which can greatly affect the performance of SIAM approach. These options are shown in Tab. 1, identified by an INB flag.

Table 1. Reservoir data for Case 1.

INB	Implicitness level
0	Well blocks implicit
1	Well blocks and wells' neighbors implicit
2	Well blocks, wells' neighbors, and the neighbors of the last gridblocks implicit

3. RESULTS

In this section, we present the comparison between the new proposed formulation and the original UTCOMP approach. Our comparison is based on two specific aspects. First, the oil and gas production rates are evaluated, in order to verify the SAIM accuracy. Second, the CPU time for both methods are compared to each other, giving the exact measurement of the achieved speed. Two case studies are used to verify the performance of proposed SAIM in conjunction with the EbFVM using triangular and quadrilateral grids. A quarter-of-five-spot configuration is used for the case studies. The first case study is a gas-flooding problem characterized by three hydrocarbon components. Tables 2 and 3 present the reservoir data and the initial and injected fluid composition, respectively, and Table 4 presents the binary interaction coefficients used in the phase behavior part of the simulator.

Table 2. Reservoir data for Case 1.

Properties	Value
Length, Width, and Height	243.84 m; 243.84 m; 60.96 m
Porosity	0.30
Initial Water Saturation	0.25
Initial Reservoir Pressure	20.65 MPa
Permeability in X, Y and Z directions	1.97×10^{-13} m²; 1.97×10^{-13} m²; 1.97×10^{-14} m²
Reservoir Temperature	299.82 K
Injection Gas Rate	5.66×10^{2} m³/d
Producer BHP	20.65 MPa

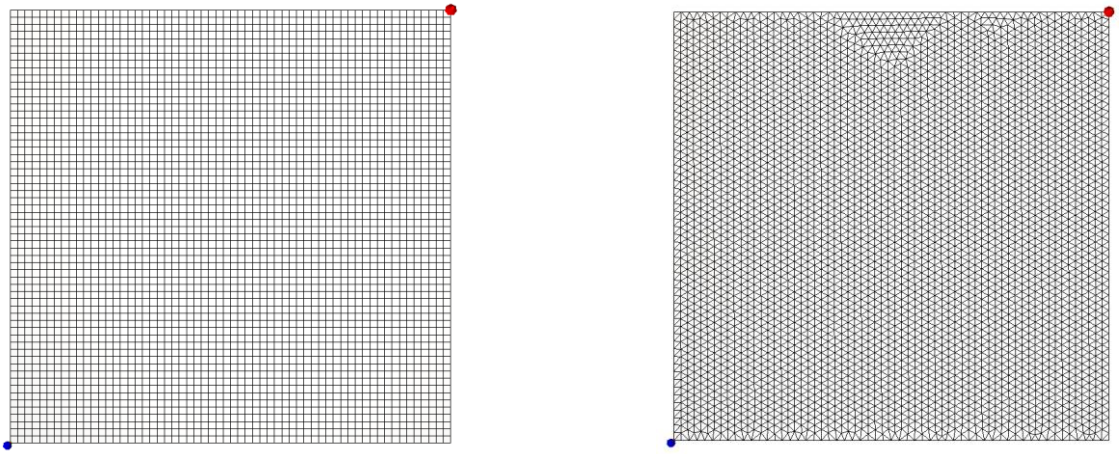
Table 3. Initial and injected fluid composition for Case 1.

Component	Initial Reservoir Composition	Injection Fluid Composition
CO_2	0.01	0.95
C1	0.19	0.05
nC16	0.80	-

Table 4. Binary interaction coefficients for Case 1.

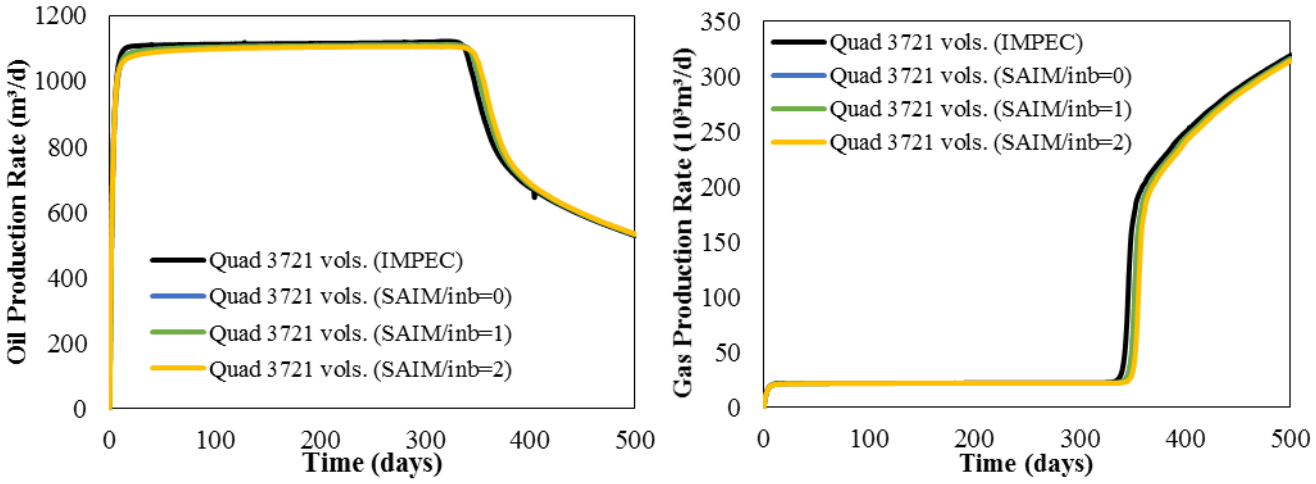
Component	CO_2	C1	nC16
CO_2	-	0.12	0.12
C1	0.12	-	-
nC16	0.12	-	-

The IMPEC and SAIM are compared for both quadrilateral and triangle element meshes, with 3721 and 3741 gridblocks, respectively. The grids for the simulations are shown in Fig. 3. Figures 4 and 5 show the results in terms of volumetric rates. From these figures, it is possible to observe a good match between the SAIM with all the three level of implicitness used and the original IMPEC formulation of the UTCOMP simulator.



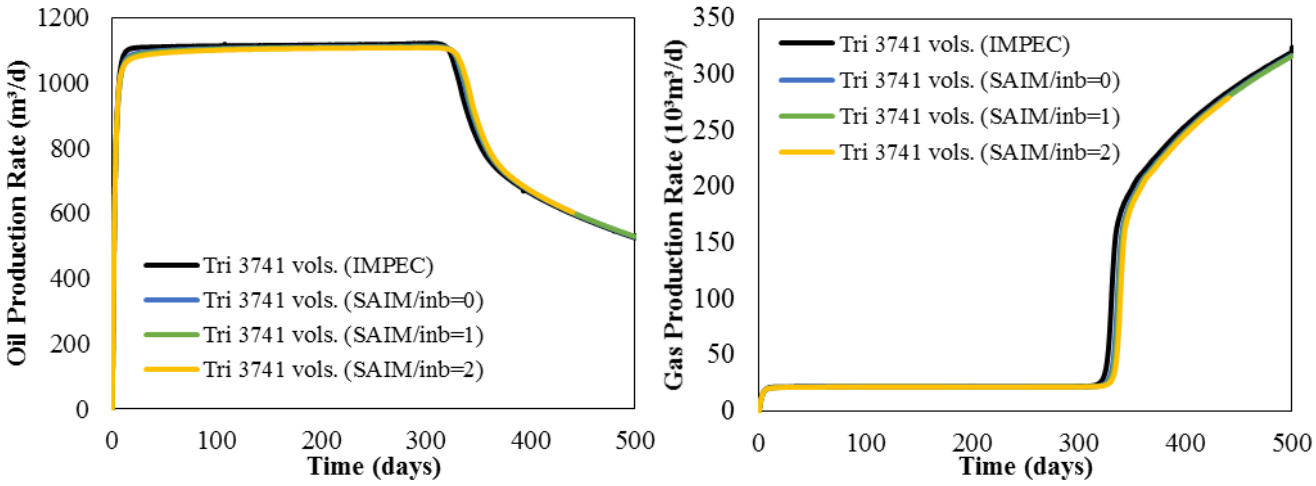
(a) (b)

Figure 3.(a) 3721-volumes quadrilateral mesh, (b) 3741-volumes triangle mesh.



(a) (b)

Figure 4. Case 1 – quadrilateral grid – 3721 vertices. (a) Oil production rate, (b) gas production rate



(a) (b)

Figure 5. Case 1 – triangular grid – 3741 vertices. (a) Oil production rate, (b) gas production rate

The comparison of the average time step and total computational times (CPU) are shown in Tables 5 and 6. The results shows the expected enhancement performance of the SAIM approach, partly caused by the higher time steps applied, especially when the implicitness level increases.

Table 5. Comparison of average time step and CPU time for quadrilateral grid - Case 1.

Formulation	Average time step (days)	CPU time (s)
IMPEC	0.02	1574.498
SAIM (inb=0)	0.06	935.938
SAIM(inb=1)	0.06	924.909
SAIM (inb=2)	0.10	576.368

Table 6. Comparison of average time step and CPU time for triangular grid - Case 1.

Formulation	Average time step (days)	CPU time (s)
IMPEC	0.03	1150.904
SAIM (inb=0)	0.06	1025.187
SAIM(inb=1)	0.08	780.816
SAIM (inb=2)	0.10	633.459

The second case study is another gas-flooding problem, again in a quarter-of-five-spot reservoir, but now characterized by six hydrocarbon components. Tables 7 and 8 present the reservoir data and the initial and injected fluid composition, respectively. For this case study, the binary interaction coefficients were set to zero. We used the same grids shown in Fig. 3 for this case study.

Table 7. Reservoir data for Case 2.

Properties	Value
Length, Width and Height	243.84 m; 243.84 m; 60.96 m
Porosity	0.35
Initial Water Saturation	0.17
Initial Reservoir Pressure	10.34 MPa
Permeability in X, Y and Z directions	1.97×10^{-14} m²; 1.97×10^{-14} m²; 1.97×10^{-14} m²
Reservoir Temperature	344.26 K
Injection Gas Rate	2.83×10^{5} m³/d
Producer BHP	8.96 MPa

Table 8. Initial and injected fluid composition for Case 1.

Component	Initial Reservoir Composition	Injection Fluid Composition
C1	0.500	0.770
C3	0.030	0.200
C6	0.070	0.010
C10	0.200	0.010
C15	0.150	0.005
C20	0.050	0.005

The oil and gas rates are shown in Figs. 6 and 7. Once again, the volumetric rates for oil and gas present a good match with those obtained with the original IMPEC approach of the UTCOMP simulator.

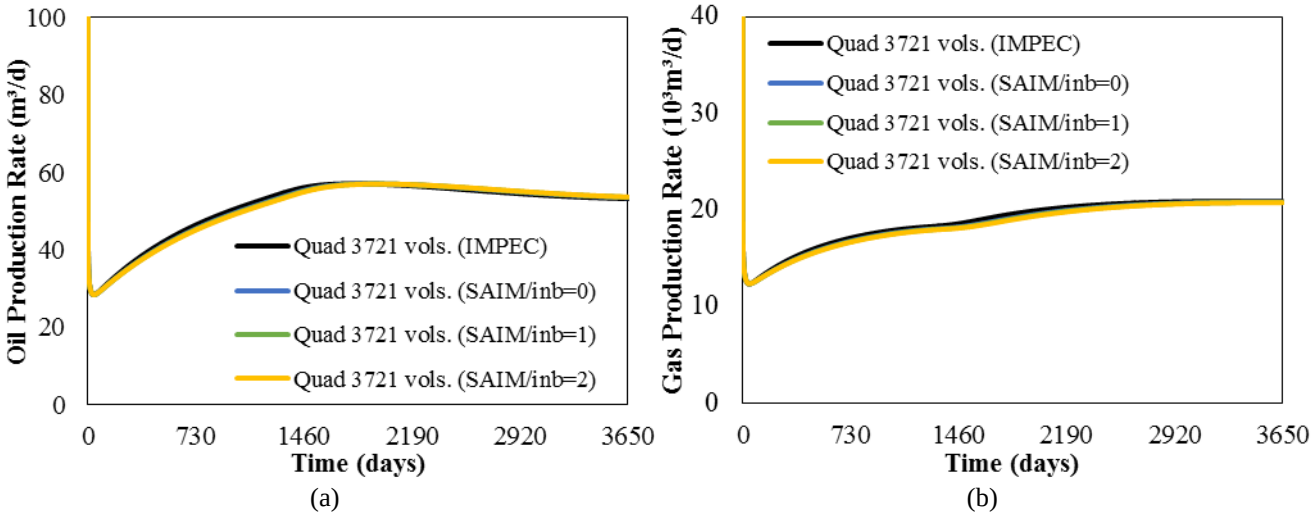


Figure 6. Case 2 – quadrilateral grid – 3721 vertices. (a) Oil production rate, (b) gas production rate

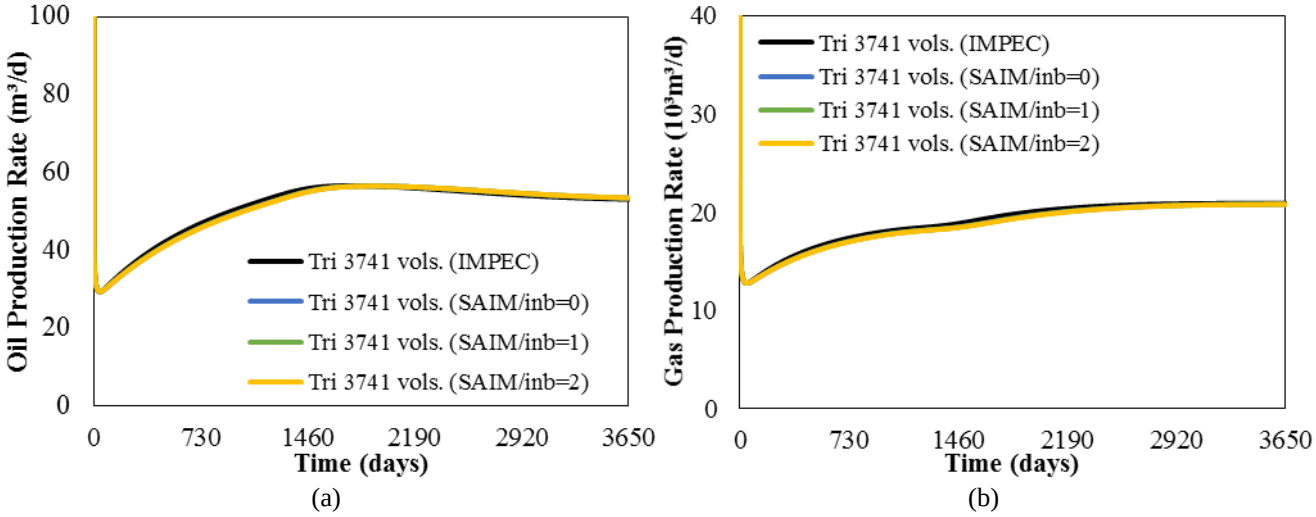


Figure 7. Case 2 – triangular grid – 3741 vertices. (a) Oil production rate, (b) gas production rate

The comparison of the average time step and CPU times are shown in Tables 9 and 10 for the quadrilateral and triangular grids, respectively. Again, the SAIM outperforms the original IMPEC present in UTCOMP in terms of average time step and CPU time, especially when the implicitness level is increased.

Table 9. Comparison of average time step and CPU time for quadrilateral grid - Case 2.

Formulation	Average time step (days)	CPU time (s)
IMPEC	0.20	1602.012
SAIM (inb=0)	0.80	1049.962
SAIM(inb=1)	1.00	848.633
SAIM (inb=2)	1.20	719.465

Table 10. Comparison of average time step and CPU time for triangular grid - Case 2.

Formulation	Average time step (days)	CPU time (s)
IMPEC	0.30	1167.009
SAIM (inb=0)	0.90	1129.291
SAIM(inb=1)	1.00	974.281
SAIM (inb=2)	1.10	889.233

4. CONCLUSIONS

The present study proposes a new formulation to combine the capabilities of two of the mostly numerical approaches used in petroleum reservoir simulation: IMPEC and FI. The proposed approach, called SAIM approach is an intermediate to an actual adaptive implicit method, commonly used in petroleum reservoir simulation. However, the static selection of FI blocks on key regions of the reservoir can enhance both the average time step and CPU time.

The next steps in this work are the expansion to three-dimensional grids, which better describe field applications, as well as the implementation of an Adaptive Implicit Method. The dynamic selection of implicit and explicit volumes tends to further improve the simulation efficiency. The framework proposed and implemented in this work is capable of receiving such features without large modifications.

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