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## **ADAPTIVE IMPLICIT METHOD APPLIED TO COMPOSITIONAL RESERVOIR SIMULATION USING UNSTRUCTURED GRIDS**

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**Abstract.** The modern oil production industry relies heavily on increasingly accurate and fast reservoir simulators. Adaptive implicit methods have, in this context, become very popular based on their ability to optimize performance by reducing the implicitness level and CPU memory usage of simulation runs. This is achieved by constantly identifying sources of numerical instability and applying the required level of implicitness in these regions, while keeping the remainder of the reservoir computed explicitly. Therefore, the main goal of the AIM approach is to reduce the size of the linear systems, but keeping the ability to reproduce the stability of the FI models, while outperforming them in terms of computational time and memory. In this work, the AIM approach is applied to compositional reservoir simulation using unstructured grids in conjunction with the Element-based Finite Volume Method (EbFVM). The results are shown in terms of saturations fields and production curves. For computational performance CPU time, time step size, and average level of implicitness are compared. The data shows relevant performance improvement without compromising the accuracy of the results.

**Keywords:** *Compositional reservoir simulation, adaptive implicit method, EbFVM, unstructured grids.*

### **1. INTRODUCTION**

One of the most important aspects of compositional reservoir simulation is choosing the appropriate algorithm or formulation to solve the system of equations, which constitute the physical model. The various formulations found in the literature can be categorized into several classes, two of the formulations that have great relevance in this work are IMPEC and FI approaches.

IMPEC (Implicit Pressure Explicit Concentration) formulations are defined by the choice to compute only pressure as a single primary variable implicit. The remaining variables are all computed afterwards, explicitly. This approach yields the smallest possible linear system of equations and, therefore, the smallest amount of computational effort per time step. However, the reduced implicitness level causes numerical instability, especially in some specific regions, as in the surroundings of wells (Collins et al., 1992). The result of this issue is a severe time step limitation for the IMPEC approach.

On the other hand, the Fully Implicit (FI) approach, as the name indicates, requires all primary variables to be solved implicitly. The Jacobian matrix then assumes a much larger size than its IMPEC version, demanding much more computational effort per time step. However, the maximum implicitness level confers much more stability for the method, eliminating most time step limitations.

The Adaptive Implicit Method (AIM) combines the advantages of both IMPEC and FI approaches. Thomas and Thurnau (1982) argued there was no need to treat an entire reservoir grid implicitly, since only small portions of the domain would actually present sources of numerical instability. They proposed a formulation in which grid volumes would be checked according to a simple criterion. If this test fails, it would be a signal of possible instability, then causing the corresponding grid blocks to be computed as FI. The remainder of the reservoir would still be calculated using the IMPEC approach.

In our work, the AIM is applied in conjunction with the Element-based Finite Volume Method using grids, which provide an efficient way to describe complex geometry reservoirs and to reduce the grid orientation effect. The IMPEC

and FI have already been compared for EbFVM grids by Fernandes (2014). Our work is entirely conducted using the UTCOMP, a multicomponent/multiphase compositional simulator developed at The University of Texas at Austin.

## 2. PHYSICAL MODEL

A compositional reservoir simulator requires basically three types of equations: material balances, physical constraints, and phase behavior. In this section, we briefly describe the most important expressions of each type.

### 2.1 Material balance

The mole balance for the hydrocarbon components is presented in Eq. (1). We should note that physical dispersion is not take into account in Eq. (1).

$$\frac{1}{V_b} \frac{\partial N_i}{\partial t} + \bar{\nabla} \cdot \left( \sum_{j=2}^{n_p} \xi_j x_{ij} \bar{u}_j \right) + \frac{\dot{q}_i}{V_b} = 0, \quad i = 1, \dots, n_c + 1 \quad (1)$$

In Eq. (1),  $V_b$  is the bulk volume,  $N_i$  represents the total amount of moles of component  $i$ ,  $\xi_j$  is the molar density of phase  $j$ ,  $x_{ij}$  is the molar fraction of component  $i$  in phase  $j$ ,  $u_j$  represents the velocity of phase  $j$ , which is given by the Darcy law,  $q_i$  is the well molar flow rate of component  $i$ , and  $n_c$  stands for the number of hydrocarbon components. The material balance for the water component is analogous to Eq. (1).

### 2.2 Pressure equation

Many constraints are required in compositional reservoir simulation. However, one of the most important is the pressure equation, which can be obtained from the volume restriction that states the total fluid volume is always equal to the pore volume. From this assumption, we obtain the following equation:

$$\left[ \phi^0 c_f - \frac{1}{V_b} \left( \frac{\partial V_T}{\partial P} \right)_{N_i} \right] \frac{\partial P}{\partial t} + \bar{V}_{tw} \bar{\nabla} \cdot (\xi_w \bar{u}_w) + \sum_{i=1}^{n_c} \bar{V}_{ti} \sum_{j=2}^{n_p} \bar{\nabla} \cdot (\xi_j x_{ij} \bar{u}_j) + \sum_{i=1}^{n_c+1} \bar{V}_{ti} \frac{\dot{q}_i}{V_b} = 0 \quad (2)$$

In Eq. (2),  $\phi^0$  is the reference porosity,  $P$  represents the pressure of the oil phase, and  $V_{ti}$  stands for the partial molar volume.

### 2.3 Phase behavior

One of the most important assumptions in our work is the local equilibrium condition. This is only true once the Gibbs free energy is minimized, which in turn leads to the fugacity constraint described in Eq. (3).

$$f_{ij} = f_{ir}, \quad i = 1, \dots, n_c; \quad j = 2, \dots, n_p (j \neq r) \quad (3)$$

The equation of State (EOS) can be used to evaluate the fugacities of each component in each hydrocarbon phase. In this work, the Peng and Robinson (1979) EOS is used to evaluate the fugacities. Further details can be found in Perschke (1988).

## 3. ADAPTIVE IMPLICIT METHOD

The concept of the AIM approach is simple. The performance limitation of the IMPEC model arises from the choice to keep the minimal implicitness level, which leads to numerical instabilities if large time steps are used. FI formulations solve this issue by solving all primary variables implicitly. As stated by Thomas and Thurnal (1982) and verified by other works, such as Collins et al. (1992), most of the reservoir grid does not require an implicit treatment at a given time level. Hence, the Adaptive Implicit Method has the responsibility of identifying which grid volumes require implicit treatment and merging all blocks into a single system of equations.

The end result of this approach is the performance enhancement, when compared to both original formulations. Relative to IMPEC model, the AIM is able to achieve time-step sizes similar to those of the FI approach, while maintaining stability and reducing the computational effort required per time level by greatly reducing the linear system size.

It is important to highlight the importance of correctly selecting the grid volumes to receive implicit treatment. The appropriate stability criterion must be defined in order to avoid leaving instabilities sources unchecked, specially given this evaluating is conducted dynamically throughout each time level. In the next sub-section, this issue is discussed in more detail.

### 3.1 Stability switch criterion

Instead of relying on a single stability test, we have implemented a combined criterion divided in two sets of analysis. The first one is inspired in the work of Thomas and Thurnau (1982). It consists of comparing the variation of phase saturations and overall molar fraction of each grid volume over the previous time level against defined threshold values. It is important to highlight that this approach lacks of a solid theoretical foundation, since there is not expression to compute the ideal thresholds and therefore, they are set arbitrarily by the user. This method, if used on its own, does not properly account for the instabilities during a simulation. However, it provides a safeguard against very large variations when combined with other tests.

The second part of the stability analysis is composed of two CFL-based tests. This switching criteria was first proposed by Russel (1989) for black oil simulations. Following, Grabenstetter applied a CFL test for compositional runs. The CFL condition can be described by the expression in Eq. (4), where  $\Delta t$  is the time step size and  $V_p$  represents the pore volume.

$$\frac{F_i \Delta t}{V_{p,i}} < 1, \quad i = 1, \dots, n_b \quad (4)$$

Additionally,  $F_i$  is a function of the flow rates, reservoir, and fluid properties. The first CFL test computes  $F_i$  as the volumetric flow of the grid block over its entire surface. Finally, the second CFL test computes the function as proposed by Coats (2001).

For this last criterion  $F_i$  is computed in two different ways. The first one accounts for the explicit treatment of compositions, as show in the following equation:

$$F_i = \max(k) \frac{Q_o \rho_o x_{o,k} + Q_g \rho_g x_{g,k}}{S_o \rho_o x_{o,k} + S_g \rho_g x_{g,k}}, \quad k = 1, \dots, n_c \quad (5)$$

In Eq. (5),  $Q$  represents the total volumetric phase flow rate, and  $\rho$  stands for the phase molar density. The second expression aims at the explicit evaluation of both relative permeabilities and capillary pressures, as shown in Eq. (6).

$$F_i = \frac{1}{2} \left| f11_i + f22_i + \sqrt{(f11_i + f22_i)^2 - 4 \det(F_i)} \right| \quad (6)$$

These tests are conducted in sequence. If a grid volume is computed as IMPEC, it has to pass all tests. If any of the above criteria is not respected, the volume becomes FI. Additionally, grid blocks containing well perforation are always set as implicit, given their special condition. More details on this implementation can be found on Drumond (2017).

## 4. RESULTS

Two case studies are presented for the accuracy and performance analysis. The comparison is performed for five formulations. The first one is the Ács et al. (1985) Implicit Pressure / Explicit Composition method, referred from now on as IMPEC. Additionally, two Fully Implicit formulations are investigated: the Ács et al. (1985) based on Fernandes (2014), and the Collins et al. (1992) formulation. These approaches will be referred as FI Acs and FI Collins. Finally, the AIM versions of the mentioned FI formulations complete the study.

The first case study is a gas flooding in a quarter-of-five-spot reservoir configuration. The reservoir fluid has 6 pseudo-components, while the injection fluid is mostly composed of lighter oil fractions. For this case, the grid presented in Fig. 1 is composed only of triangular elements with 11,622 nodes (control volumes). The reservoir data and initial reservoir fluid and injection fluid compositions are given in Tabs. 1 and 2, respectively.

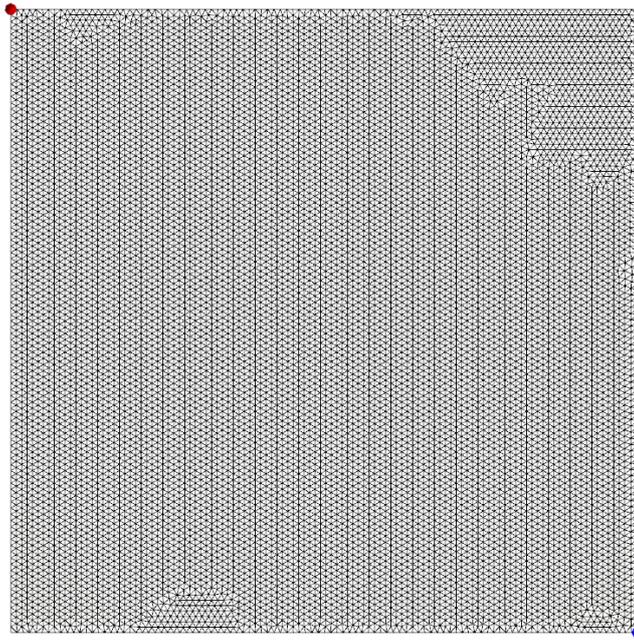


Figure 1. Triangular elements grid composed of 11,622 volumes.

Table 1. Reservoir properties – Case study 1.

Property	Value
Porosity	0.35
Initial Water Saturation	0.17
Initial Pressure	10.34 MPa
Permeability (X, Y and Z)	$9.86 \times 10^{-15} \text{ m}^2$ , $9.86 \times 10^{-15} \text{ m}^2$ , $9.86 \times 10^{-15} \text{ m}^2$
Temperature	344.26 K

Table 2. Initial reservoir fluid and injection fluid compositions – Case study 1.

Component	Initial reservoir composition	Injection composition
C1	0.50	0.77
C3	0.03	0.20
C6	0.07	0.01
C10	0.20	0.01
C15	0.15	0.005
C20	0.05	0.005

Figure 2 shows the oil and gas production rates for the AIM and FI approaches. From this figure, we can clearly observe a good match of the production curves obtained for all the approaches used.

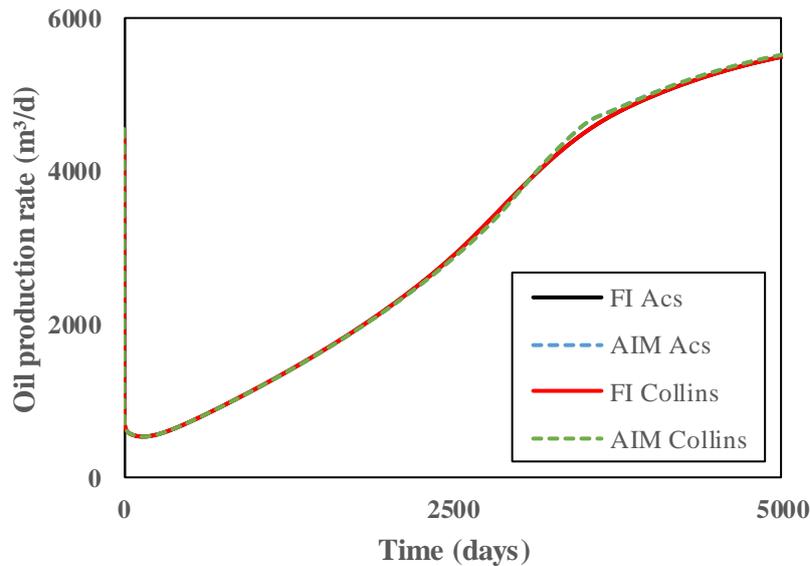


Figure 2. Oil production rate for case study 1.

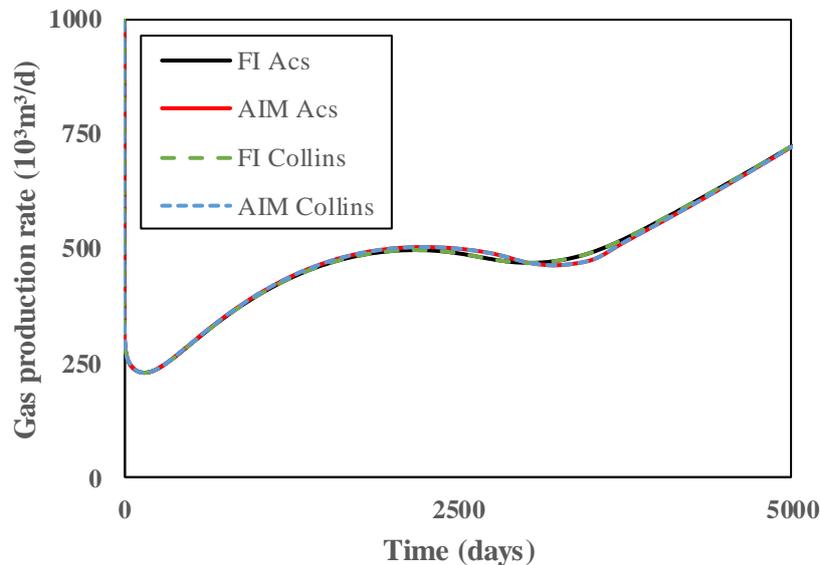


Figure 3. Gas production rate for case study 1.

The computational performance and other important parameters of the simulation for this case study are presented in Tab. 3. From Tab. (3), it is clear that the AIM and FI methods have similar performance in terms of average time step and total number of Newton iterations. However, the adaptive methods greatly outperform their FI counterparts, while kept only a small percentage of the control volumes implicit. The IMPEC, the severe time step limitations produced an unpractical solution in terms of computational performance. Therefore, we do not present the results of this formulation in Tab. 3.

Table 3. Performance comparison – Case study 1.

Formulation	Average DT (days)	N° of iterations	FI%	CPU time (s)
IMPEC	-	-	0.00	FAILED
FI Acs	17.42	654	100.00	1400.96
FI Collins	17.42	603	100.00	1043.21
AIM Acs	16.07	636	6.12	580.11
AIM Collins	16.18	634	5.29	456.79

Figure 4 shows the gas saturation front at 5,000 days obtained with the AIM Acs and AIM Collins formulations. From this figure, we can clearly observe a good match of gas saturation field produced by both AIM approaches. Fig. 5

presents the implicitness fields at 5,000 days from the two aforementioned AIM approaches, in which the red regions represent implicit treated volume grids. Likewise, the gas saturation field the implicitness field of both AIM approaches are very similar. It is also important to stress that only the region around the wells were selected as FI.

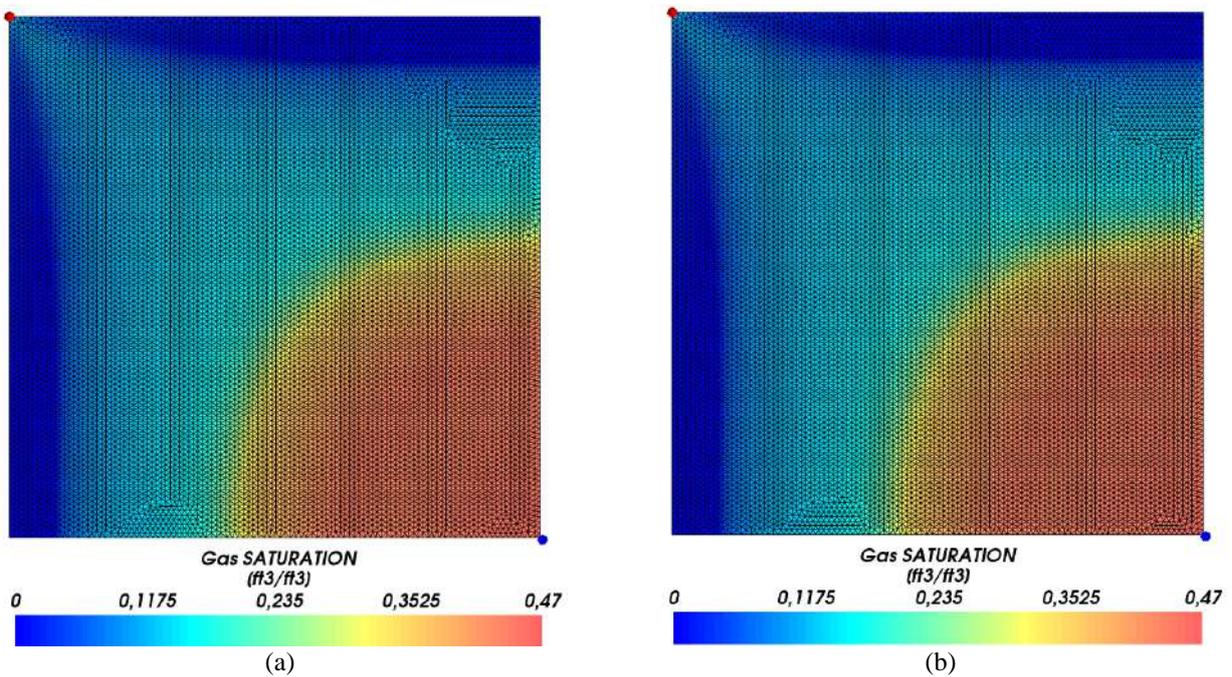


Figure 4. Gas saturation profiles at 5,000 days – Case study 1. (a) AIM Acs and (b) AIM Collins

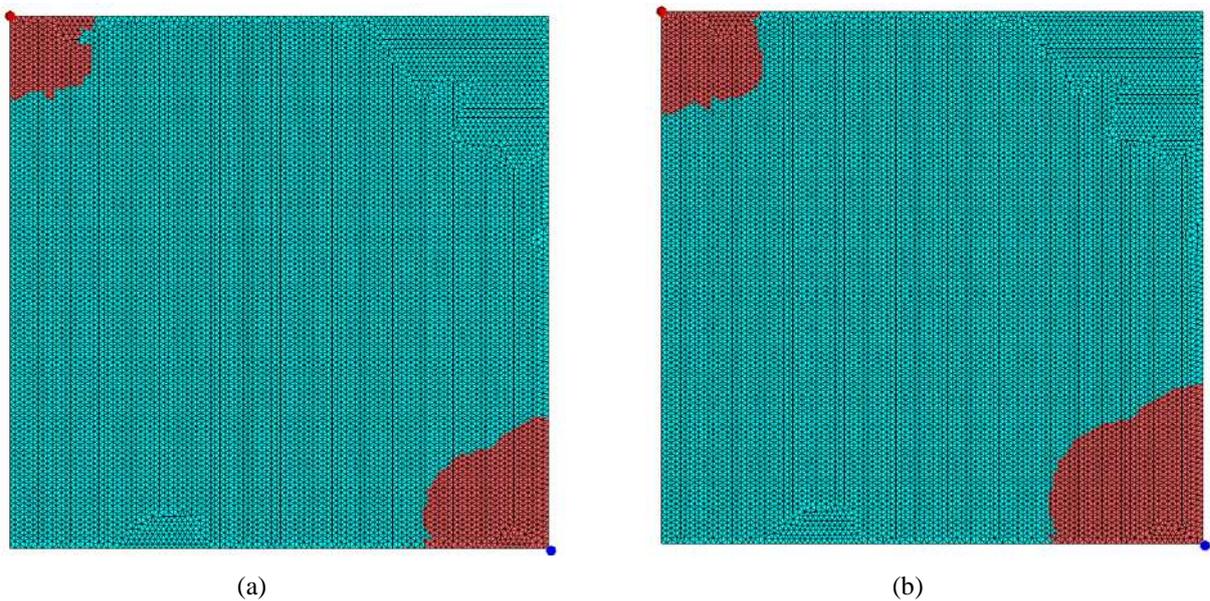


Figure 5. Implicit gridblocks distribution at 5,000 days – Cases study 1. (a) AIM Acs and (b) AIM Collins

The second case study is also a gas flooding problem, but now the reservoir is characterized by 3-pseudo-components with the fluid rich on heavier oil fractions. A five-spot reservoir configuration is discretized with a grid composed of only quadrilateral elements with 32,925 nodes (control volumes). Additionally, the reservoir presents a heterogeneous field for both x and y permeabilities. The grid and the absolute permeability field in x- and y-directions is presented in Fig. 6. The reservoir data and in-place and injected fluid compositions are given in Tabs. 4 and 5, respectively.

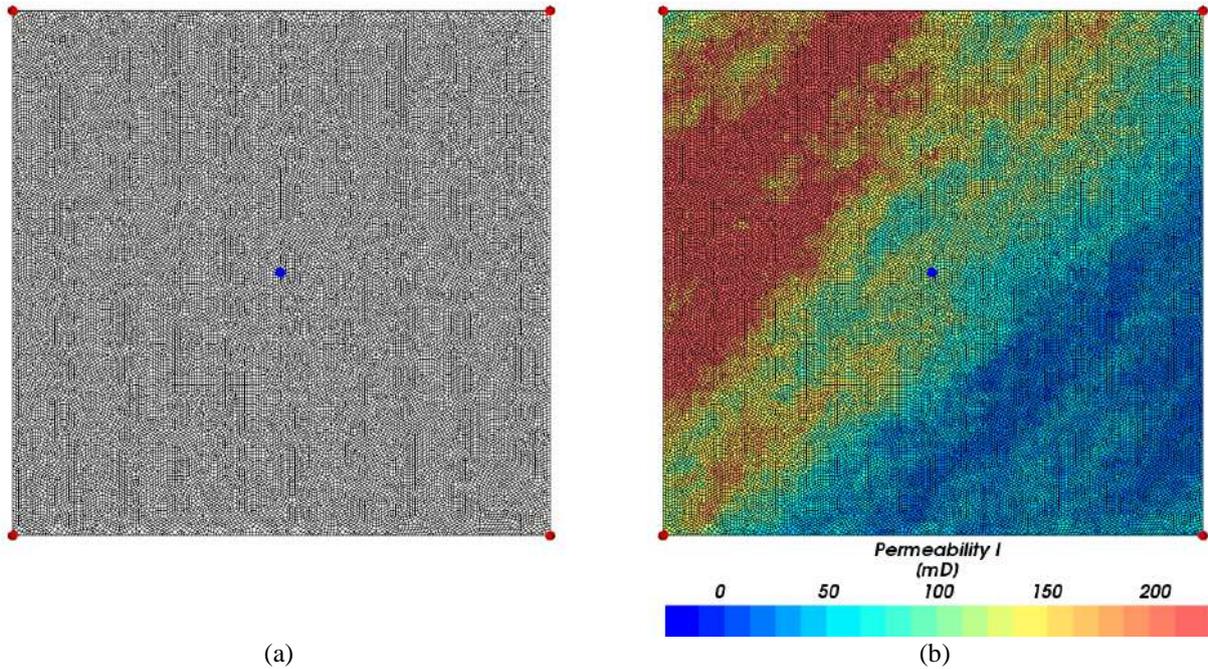


Figure 6. Quadrilateral elements grid composed of 32925 volumes (a) and permeability field (b).

Table 4. Reservoir properties – Case study 2.

Property	Value
Porosity	0.35
Initial Water Saturation	0.25
Initial Pressure	20.68 MPa
Temperature	299.82 K

Table 5. Reservoir and injection fluid compositions – Case study 2.

Component	Initial reservoir composition	Injection composition
CO <sub>2</sub>	0.01	0.95
C1	0.19	0.05
NC16	0.80	0.00

Figs. 7 and 8 show the production curves for the case 2. Likewise case 1, the production curves obtained with the AIM and the FI approaches are in good agreement. Again, the IMPEC approach was not able to perform the simulation with reasonable time-step sizes.

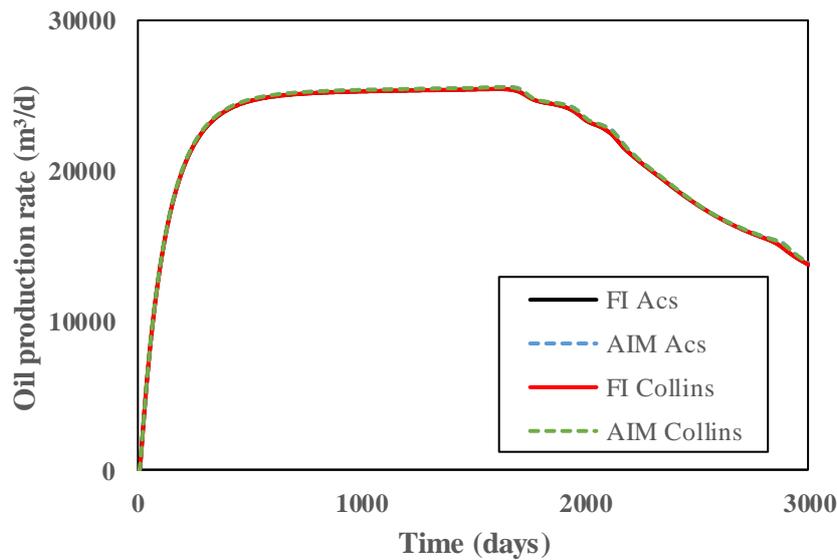


Figure 7. Oil production rate for case study 2.

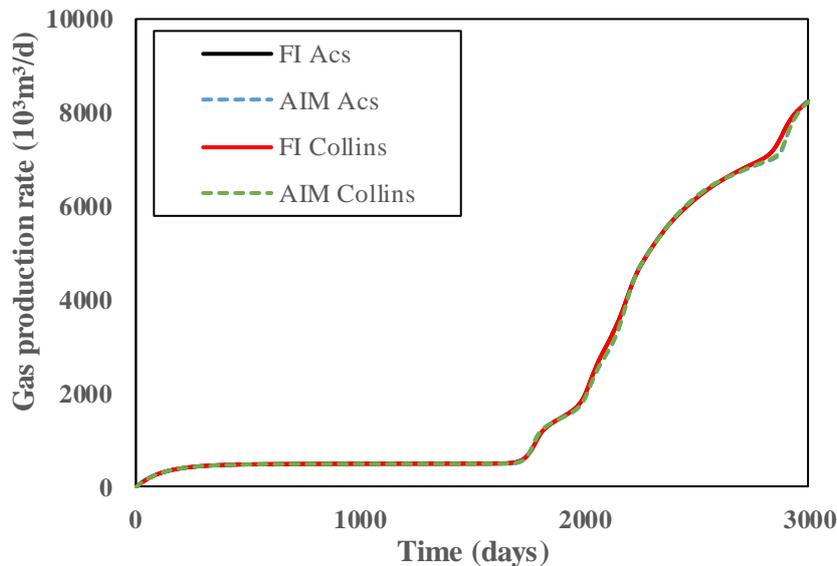


Figure 8. Gas production rate for case study 2.

The Computational performance and other important parameters of the simulation for case study 2 is presented in Tab. 6. From this table, we can verify that the AIM greatly outperforms the FI formulations. Additionally, it is important to highlight that the AIM results were obtained while requiring only around 10% of the grid blocks to be computed implicitly. These data reinforce the initial assertion of this work that, in general, just few areas of the reservoir need to be considered as FI in order to eliminate the numerical instabilities and time-step size limitations.

Table 6. Computational performance – Case study 2.

Formulation	Average DT (days)	N° of iterations	FI%	CPU time (s)
IMPEC	-	-	0.00	FAILED
FI Acs	5.04	1749	100.00	5545.64
FI Collins	4.84	1772	100.00	5527.17
AIM Acs	3.88	2141	8.90	2401.40
AIM Collins	3.99	1854	12.80	1636.38

Figs. 9 and 10 present the gas saturation and the implicitness fields at 3,000 days using the two AIM approaches. The gas saturation field obtained with both AIM Acs and Collins approaches are in good agreement. However, when the implicitness fields are compared in Fig. 9, it is possible to see the AIM Collins has much more implicit volumes at

the end of the run. However, as shown in Tab. (6), this works as advantage to the method in comparison with AIM Acs. This shows a smaller number of implicit blocks does not necessarily mean a faster simulation. The goal of the switching criterion is to properly identify instability sources and treat them accordingly.

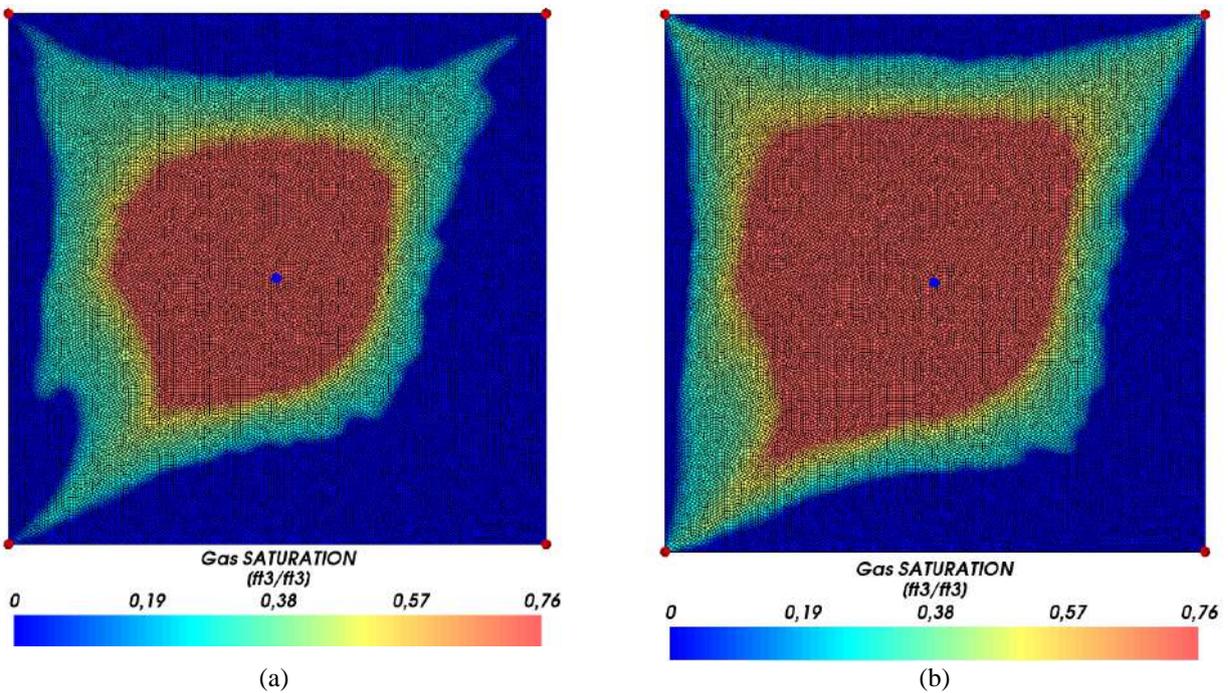


Figure 9. Gas saturation field 3,000 days – Case study 2. (a) AIM Acs and (b) AIM Collins

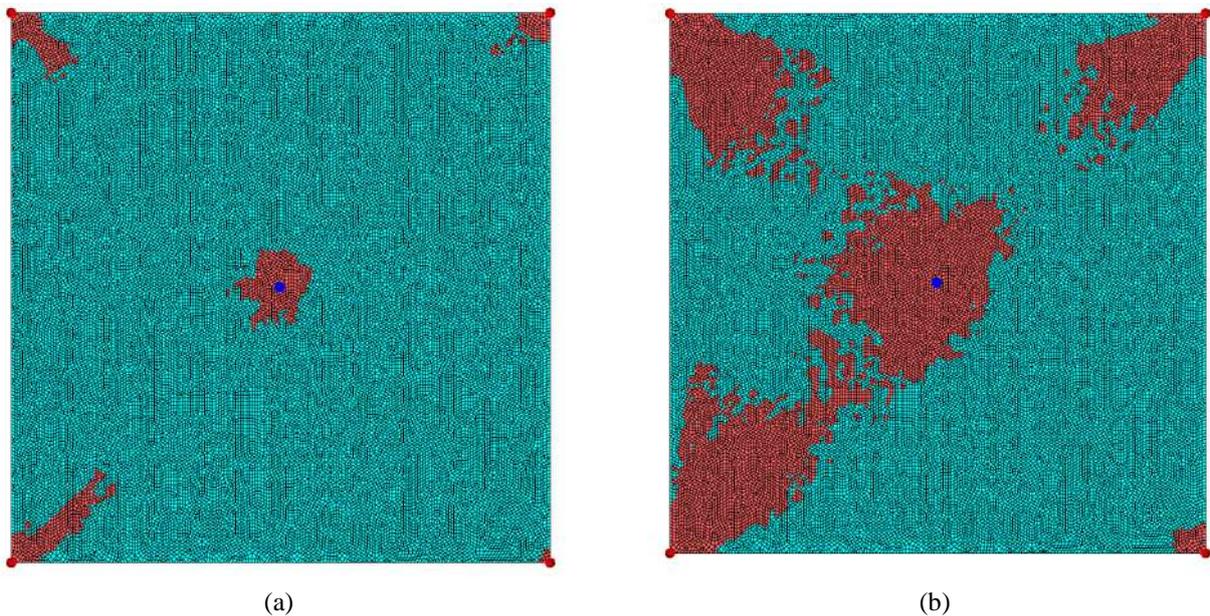


Figure 10. Implicit gridblocks distribution at 3,000 days – Case study 2. (a) AIM Acs and (b) AIM Collins

## 5. CONCLUSIONS

In this work, two AIM formulations were implemented using 2D unstructured grids in conjunction with the Element-based Finite Volume Method. The comparison with IMPEC and FI formulations shows the AIM implemented approaches are capable of producing accurate results, while providing significant improvement in the computational performance. Additionally, by not requiring the entire mesh to be implicitly computed, the AIM reduces the computer memory requirements, allowing the simulation of reservoir with large grid sizes. The AIM approaches in conjunction with unstructured grids using the EbFVM is currently undertaken.

## 6. ACKNOWLEDGEMENTS

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