AN ADAPTIVE APPROACH FOR COMPOSITIONAL RESERVOIR SIMULATION IN CONJUCTION WITH UNSTRUCTURED GRIDS

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Abstract. *One of the key aspects of compositional reservoir simulation is the algorithms or formulations used to solve the equations for modeling fluid flow in the permeable media. Basically, the main goal is to have algorithms that produce accurate results with efficient computational times, while maintaining computational stability for different recovery processes. A literature survey shows that several approaches have been developed in the last decades. The formulations are different partly by the choice of primary variables and implicitness level used to solve the governing equations. Implicit Pressure, Explicit Composition (IMPEC) models treat a single variable implicitly, reducing the run time for each time step, while becoming more vulnerable to numerical instabilities. On the other hand, Fully Implicit (FI) schemes evaluate all primary variables implicitly, which results in a greater stability but more expensive per time level and more memory consumption. Herein, we present a dual approach that combines advantages of fully implicit and IMPEC approaches. The*

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proposed model combines the two formulations into an adaptive method with variable level of implicitness throughout the reservoir. If the computations for an IMPEC gridblock is unstable or requires an excessively small time-step, then that gridblock is switch to FI. On the other hand, if the sources of instabilities, as in the saturation front, are not present anymore in a FI gridblock, we switch the computations in that gridblock to IMPEC. We use the CFL (Courant-Friedrichs-Lewy) number and a threshold value based on a saturation variation as switching criteria to change computations in a gridblock from IMPEC to FI and vice-versa. The main novelty of this work is the association of this Adaptive Implicit Method with the Element based Finite Volume Method scheme for unstructured meshes. The results are shown in terms of oil and gas production rate curves and CPU time.

Keywords: *Compositional reservoir simulation, Adaptive Implicit Method, EbFVM, Switch criteria*

1 INTRODUCTION

The relevance of the oil and gas industry is widely known in all sectors of economy. The final products of this industry are used in large scale on an enormous variety of fields that explains the huge amount of investment in this area. An expected consequence is the impact on global markets. For decades, the economy has been profoundly affected by the result of political events on oil prices.

Given this scenario, it comes with no surprise that petroleum production has attracted the attention of companies and research groups in a continuous effort to improve efficiency and reduce risks. Evaluating the entire petroleum industrial chain, oil production is probably the step where more uncertainties exist. The advent of computational simulation produced an impact in this area since such a tool enabled a much faster increase on effectiveness in a few decades than before. Reservoir simulation has become a key instrument for companies analyzing new and old prospects as well as academic researchers studying new production processes.

The currently available reservoir simulators have reached a great level of accuracy and now such simulators can handle several recovery processes, from the most traditional ones to the most recently developed. Then, a large amount of effort has been directed into computational efficiency. Simulating real field applications demands large amounts of processing power and storage capacity, leading to large computational times. The present work means to tackle this issue on a simulator already available with several formulations. Our approach consists in combining two of these algorithms into a new method for a performance improvement requiring few changes on the simulator framework.

The first goal of this work is to implement and verify the advantages of an Adaptive Implicit Method (AIM) in comparison with the Ács et al. (1958), Implicit Pressure, Explicit Composition and the Fernandes (2014), Fully Implicit formulations. Herein, we combine the aforementioned methods in order to have the AIM approach. The AIM approach was applied to the UTCOMPRS simulator from the University of Texas at Austin. UTCOMP is a multicomponent/multiphase compositional equation-of-state simulator, which can handle the simulation of several enhanced oil recovery processes. Two-dimensional case studies involving gas flooding problems are applied to several reservoir geometries. We should note that different fluid properties give rise to very distinct problems concerning the phase behavior and hence leads to examining how various numerical schemes perform.

An important issue when working with the AIM approach is the switching criteria to change a grid cell from IMPEC to FI or vice-versa. A weak criteria algorithm cannot effectively determine any performance improvement and as a result it can produce instabilities. Therefore, another objective of the present study is to implement and test two available switch criteria from the literature. All comparisons are first carried out for both criteria in order to understand their behavior in various scenarios. Finally, we are going to combine both criteria aiming to improve the performance of the AIM approach. The new AIM approach presented in this work will be implemented in conjunction with the Element-based Finite Volume Method (EbFVM) using unstructured grids. The results will be presented in terms of oil and gas producing rates, and CPU time.

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2 GOVERNING EQUATIONS

In this section we present the main model equations concerning the material balances, constraint equations, and phase behavior that are involved in a compositional model.

2.1Material balances

Neglecting the mass transfer between the water and hydrocarbon phases and the physical dispersion of the components, and assuming phase velocities are modelled by Darcy law for multiphase flow, and no chemical reactions take place in the porous media, the material balance for the hydrocarbon and water components are given by

$$\frac{1}{V_b}\frac{\partial N_i}{\partial t} = \vec{\nabla}\cdot\sum_{j=1}^{n_p}\lambda_j\xi_j x_{ij}\,\overline{\overline{k}}\cdot(\vec{\nabla}P+\vec{\nabla}P_{cj}-\gamma_j\,\vec{\nabla}D)+\frac{q_i}{V_b},\quad i=1,...,n_c+1,\ \ j=1,...,n_p \tag{1}$$

In Eq. (1), V_b is the bulk volume, N_i denotes the number of moles of component i, t represents time, n_c and n_p are the number of hydrocarbon components and phases, respectively, λ_j is the phase mobility, ξ_j stands for the phase molar density, x_{ij} is the molar fraction of component i in phase j, K denotes the absolute permeability tensor, P is the oil pressure, P_{cj} is the capillary pressure between phase j and oil phase, γ_j represents the specific gravity of phase j, D stands for the reservoir depth which is positive in downward direction, and q_i denotes the source/sink term of component i due to the producing/injecting well.

2.2 Constraint equations

Many constraint expressions are applied to the model. Herein, we limit ourselves to show the most important one: the pressure equation. Ács et al. (1985) obtained the pressure equation from a volumetric restriction. From this constraint, we can state that the total amount of fluid should be equal to the available pore volume, which can be written as

$$V_t(P,\vec{N}) = V_p(P) \tag{2}$$

In Eq. (2), V_t is the total volume of fluid, V_p represents the pore volume and $\vec{N}$ is the component moles vector. Taking the derivatives with respect to time in both sides of Eq. (2) and assuming porosity is a weak function of pressure, we obtain the following equation for pressure:

$$\left(V_p^0 c_f - \frac{\partial V_t}{\partial P}\right)\left(\frac{\partial P}{\partial t}\right) - \sum_{i=1}^{n_c+1} \overline{V}_{ti} \vec{\nabla} \cdot \sum_{j=1}^{n_p} \lambda_j \xi_j x_{ij} \overline{\overline{k}} \cdot \vec{\nabla} P = \sum_{i=1}^{n_c+1} \overline{V}_{ti} \vec{\nabla} \cdot \sum_{j=1}^{n_p} \lambda_j \xi_j x_{ij} \overline{\overline{k}} \cdot (\vec{\nabla} P_{cj} - \gamma_j \vec{\nabla} D) + \sum_{i=1}^{n_c+1} \overline{V}_{ti} q_i \tag{3}$$

The c_f denotes the compressibility factor, and $\overline{V}_{ti}$ is the total volume derivative with respect to component *i*.

2.3 Phase behavior

There are two aspects to the phase behavior calculation. The first one concerns the phase equilibrium. In this work, we assume local phase equilibrium in the reservoir, which can be guaranteed by

$$f_{ij} = f_{ir}, \quad i=1,...,n_c, \quad j=2,...,n_p (j \neq r) \tag{4}$$

Equation (4) basically states the component fugacity (*f*) has to be the same in all phases for an equilibrium to be stablished. For a given set of phases, their compositions and, consequently, properties are computed using the Peng and Robinson (1976) equation of state for multicomponent systems as presented by Perschke (1988).

$$P = \frac{RT}{v-b} - \frac{a}{v(v+b)+b(v-b)} \tag{5}$$

In Eq. (5), *T* is the temperature, *R* denotes the universal gas constant, *v* represents the specific volume. Finally, *a* and *b* are the equation of state parameters.

2.4 ELEMENT-BASED FINITE VOLUME METHOD

The Element-based Finite Volume Method, from now referred as EbFVM, was introduced by Baliga and Patankar (1980) and Raw (1985) using triangular and quadrangular grids, respectively in the context of computational fluid dynamics, and received the later denomination by Maliska (2004). The EbFVM produces flexible unstructured grids able to handle extremely complex geometries when compared to Cartesian and Boundary Fitted discretizations. The latter can actually handle some irregularities, but only to a certain degree (Heinemann et al., 1989).

In the EbFVM approach, we first divide the reservoir geometry in elements. These entities, for 2D grids, can assume the triangular or quadrilateral shapes or a mix of them as presented in Fig. 1. In this figure, the thick lines define the elements, while the dashed lines present their division in sub-elements. These entities are also called sub-control volumes (scv) because the conservation equations are integrated for each sub-element. The grid volumes are formed, around each node, by assembling all sub-control volumes that share the same node. Therefore, we can easily verify that we still have a conservative approach, that borrows from finite element

method the idea of elements and shape functions. In order to generalize, the shape functions are commonly written in the computational plane, where the element shape is all regular no matter the element is distorted in the physical plane. Figure 2 shows the triangular and quadrangular elements in the physical and computational planes.

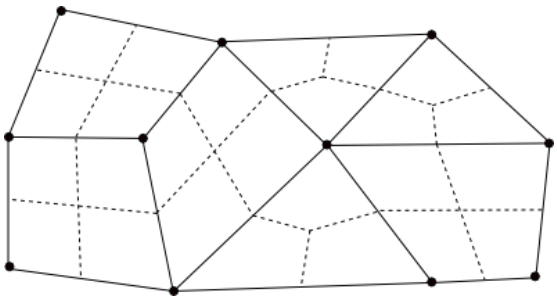

Figure 1. EbFVM grid

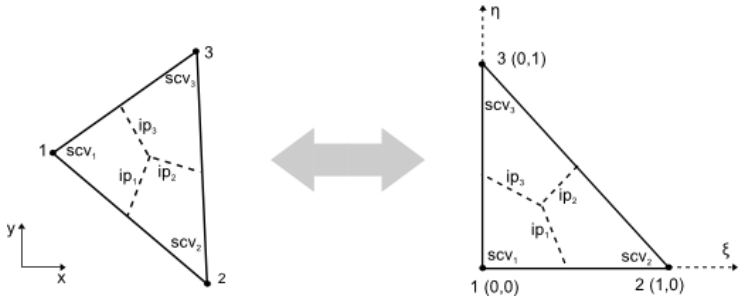

Figure 2. Two-dimensional triangular element transformation

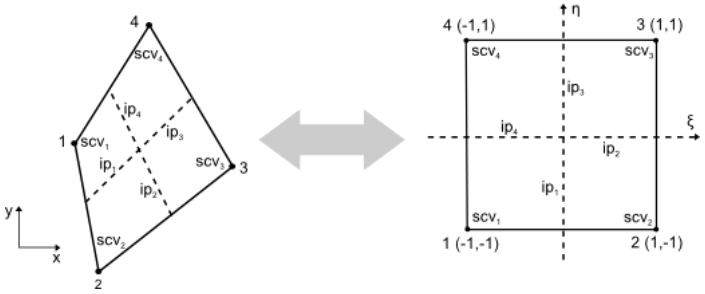

Figure 3. Two-dimensional quadrilateral element transformation

The relationship between the actual elements, in the physical plane, and their transformed, or computational, versions is stablished by the shape functions. The shape functions can be used to compute properties at any point inside the element, as well as the derivatives. They are shown for the triangular and quadrilateral elements, respectively, in Eqs. (6) and (7).

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$$\tilde{N}_1(\xi,\eta) = 1-\xi-\eta; \quad \tilde{N}_2(\xi,\eta) = \xi; \quad \tilde{N}_3(\xi,\eta) = \eta \tag{6}$$

$$\begin{aligned} \tilde{N}_1(\xi,\eta) &= \frac{1}{4}(1-\xi)(1-\eta); \quad \tilde{N}_2(\xi,\eta) = \frac{1}{4}(1+\xi)(1-\eta) \\ \tilde{N}_3(\xi,\eta) &= \frac{1}{4}(1+\xi)(1+\eta); \quad \tilde{N}_4(\xi,\eta) = \frac{1}{4}(1-\xi)(1+\eta) \end{aligned} \tag{7}$$

In the expressions above $\tilde{N}_i$ represents the shape function of each element node, while η and ξ are the coordinates in the computational plane. Further details about the EbFVM applied to 2D compositional reservoir simulation can be found in Marcondes and Sepehrnoori (2010).

3 ADAPTIVE IMPLICIT METHOD

The Adaptive Implicit Method (AIM), the subject of this work, arises as combination of two different types of formulations. The first one, Implicit Pressure/Explicit Composition (IMPEC) is defined by solving only pressure implicitly and the rest of primary variables explicitly. In general, this approach presents severe time-step size limitation due to stability issue, but the computational time per time-step is inexpensive, since only the pressure equation is solved implicitly. The Fully Implicit (FI) models, on the other hand, computes all primary variables implicitly giving rise to a block Jacobian matrix, which requires much more computational effort per time step. In general, the additional computational effort is balanced by the larger time-steps applied to FI simulations, since FI is much more stable than IMPEC approach.

For this work, these methods are already developed for the same physical modeling and discretization method presented in the previous works. The main goal of the AIM is to combine the advantages of both approaches, while mitigating their shortcomings. As stated by Thomas and Thurnal (1983), only a small fraction of the grid volumes are responsible for the instabilities observed in the IMPEC approaches. These instabilities occur mainly in the region of large flow rates, like for instance, close to the wells and saturation front. Therefore, the idea is to turn the gridblocks that are unstable with the use of large time-step to FI and keep the rest of the reservoir with the IMPEC approach. Additionally, treating only a part of the reservoir implicit makes the linear system smaller than the FI version, reducing the required computational effort per time step. In order to achieve this task, we need a better understanding of the formulations advantages and issues.

3.1 Jacobian evaluation

The Jacobian matrix for the AIM approach assumes an intermediate size between the IMPEC and FI approaches. However, it is relevant to understand how we can assemble the

Jacobian matrix for the AIM approach. Let us use the coarse grid shown in Fig. 4 for the purpose of illustration.

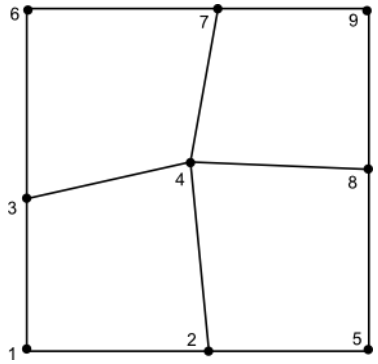

Figure 4. EbFVM grid with 9 nodes

For the grid presented in Fig. 4, only nodes 1 and 9 will be evaluated through a FI approach. All the remaining nodes are evaluated through an IMPEC approach. Taking into account three hydrocarbon components plus water component, the original linear system is given in Fig. 5. The Jacobian entries are, for this case, 5x5 submatrices. Each line of the square denotes the equation for a primary variable in a given node. The x's in the squares mean non-null coefficients. Considering the first line of squares, we can verify that only the first square is full and the ones related to gridblocks two, three and four, only the first column has non null coefficients. This column refers to the pressure coefficients that are treat implicitly in the IMPEC approach.

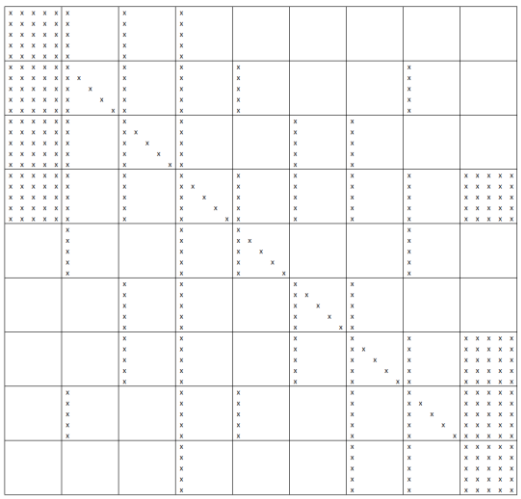

Figure 5. Full Jacobian matrix

If we look at the second line of squares, we can verify that except for the pressure coefficients (first non null column), the rest of the block is diagonal. This will allow us to remove the lines from second to last one of this line of square. Performing this operation, for all lines of squares related to IMPEC gridblocks, we obtain the following reduced Jacobian matrix:

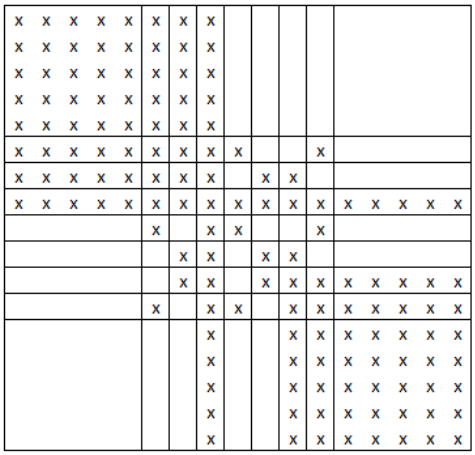

Figure 6. Reduced Jacobian matrix

The reduced Jacobian matrix presented in Figure 6 is clearly smaller than the one shown in Fig. 5. After solving, the implicit unknowns, we obtain the explicit unknowns using the lines removed from full Jacobian matrix in Fig. 5.

3.2 Switching criteria

One of the major issues regarding the AIM approach refers to the way the gridblocks are selected as FI or IMPEC. This is no simple task, since the instability conditions will change as the simulation proceeds. In other words, it is not possible to guarantee that a given gridblock regarded as IMPEC at the beginning of the simulation will conserve this property for the whole simulation.

A switching criterion must then be stablished to verify whether or not each gridblock is a potential source of instability. For instance, if at any given time level, a certain gridblock treated as IMPEC is identified as a possible source of instability, then it becomes FI until another test shows that this condition no longer exists.

Two switching criteria were implemented for this study: the threshold and CFL criteria. The Threshold criterion was proposed by Thomas and Thurnal (1983) for black-oil model. It consists of setting a limit for the phase saturations changes over a time level. If any phase saturation for a gridblock exceeds this threshold value, the block must be treated FI. Setting the threshold value is, as stated by Thomas and Thurnal (1983), performed by a preliminary trial-and-error procedure, until an optimal limit is verified. This is the major shortcoming of this criterion, which can severely undermine its efficiency.

The second switching criterion is based on the work of Coats (2001), which uses the CFL (Courant-Friedrichs-Lewy) as the CLF stability criterion. This criterion can be state as

$$\frac{F_i \Delta t}{V_{p,i}} < 1, \quad i=1,\ldots,n_b \tag{8}$$

In Eq. (8), Δt represents the time step size, $V_{p,i}$ is the pore volume of each gridblock, and n_b stands for the number of gridblocks. The F_i is a function of the flow rates, reservoir and fluid properties. Basically, if the condition in Eq. (8) is observed, the gridblock is stable and it can be evaluated explicitly. Otherwise, the FI approach is necessary. Coats (2001) proposed two ways to compute F_i. The first one aims at the explicit evaluation of relative permeabilities and capillary pressures, while the other one focus on the explicit compositions. The expressions for both calculation modes are given by

$$F_i = \frac{1}{2} \left| f11_i + f22_i + \sqrt{(f11_i + f22_i)^2 - 4det(F_i)} \right|, \quad i=1,...,n_b \tag{9}$$

$$F_i = Max(k) \frac{Q_o \rho_o x_{ok} + Q_g \rho_g x_{gk}}{S_o \rho_o x_{ok} + S_g \rho_g x_{gk}}, \quad k=1,...,n_c \tag{10}$$

In Eq. (9), the f_{ij} terms are functions of phase mobilities, phase saturations, transmissibilities, and capillary pressures. In Eq. (10), Q are the total volumetric flow rates through each interface, and ρ represent the phase mass densities. More details about these expressions can be found in Coats (2001). Once F_i is computed by both equations, the highest value is selected for the stability test.

4 RESULTS

Two case studies are selected for the AIM comparison against the FI and IMPEC formulations. As mentioned before, the results are presented in terms of accuracy of production curves and CPU performance.

4.1 Case 1: two-dimensional irregular grid

For this first case study, we apply a 2D grid for an irregular-shaped reservoir composed solely of triangular elements. The reservoir fluid is characterized by 6 pseudo components, while the injection fluid is constituted primarily by light hydrocarbon fractions. There are two producer wells and a single injector well. All the reservoir and fluid data are presented in Tables. 1 through 5.

Table 1. Reservoir data for Case study 1

Property	Value
Initial water saturation	0.17
Initial Pressure	10.34 MPa
Formation temperature	344.26 K

Table 2. Fluid composition data for Case study 1

Component	Initial Reservoir Composition	Injection Fluid 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

Table 3. Component data for Case study 1

Component	P_c (MPa)	T_c (K)	v_c (m^3/kmol)	MW (kg/kmol)	Ac. Factor
C1	4.60	190.60	$9.99x10^{-2}$	16.04	0.022
C3	4.25	369.83	$2.00x10^{-1}$	44.10	0.152
C6	3.01	507.44	$3.70x10^{-1}$	86.20	0.301
C10	2.10	617.67	$6.30x10^{-1}$	142.30	0.488
C15	1.38	705.56	1.04	206.00	0.650
C20	1.12	766.67	1.34	282.00	0.850

Table 4. Operational conditions data for Case study 1

Operational condition	Value
Constant gas rate injection	$2.83x10^4$ m^3/d
Producer's bottom hole pressure	8.96 MPa

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Table 5. Binary interaction coefficient data for Case study 1

Component	C1	C3	C6	C10	C15	C20
C1	-	-	-	-	0.05	0.05
C3	-	-	-	-	0.005	0.005
C6	-	-	-	-	-	-
C10	-	-	-	-	-	-
C15	0.05	0.005	-	-	-	-
C20	0.05	0.005	-	-	-	-

Figure 6 shows the reservoir that contains three wells with 27,271 gridblocks. The red dots indicate the producer wells and the injector is represented by the blue dot. In order to provide more complexity and the simulation be closer to a real application, we used a heterogeneous absolute permeability and porosity fields based on real field applications, as shown in Figs. 7 and 8.

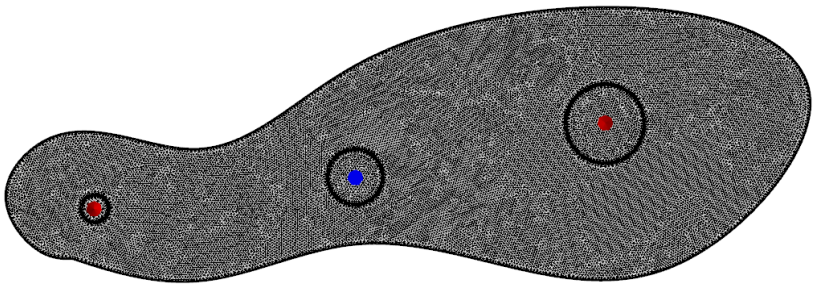

Figure 6. A two-dimensional grid with 27,271 gridblocks

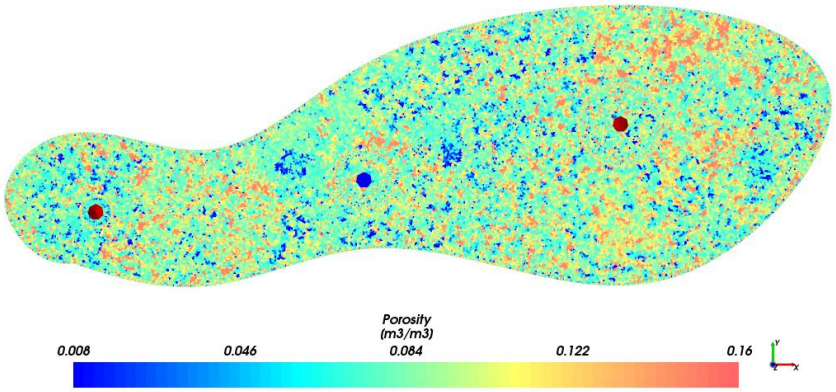

Figure 7. Porosity field for case 1

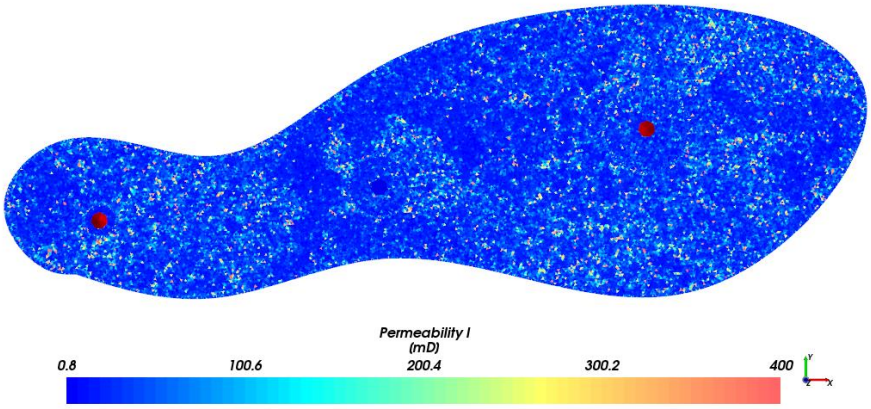

Figure 8. X and Y permeability field for case 1

The oil and gas production curves are first displayed for a 300-days simulation time. No production curve is shown for the IMPEC formulation, since the IMPEC approach did not converge for this heterogeneous case, although several attempts to adjust the simulation parameters were tried.

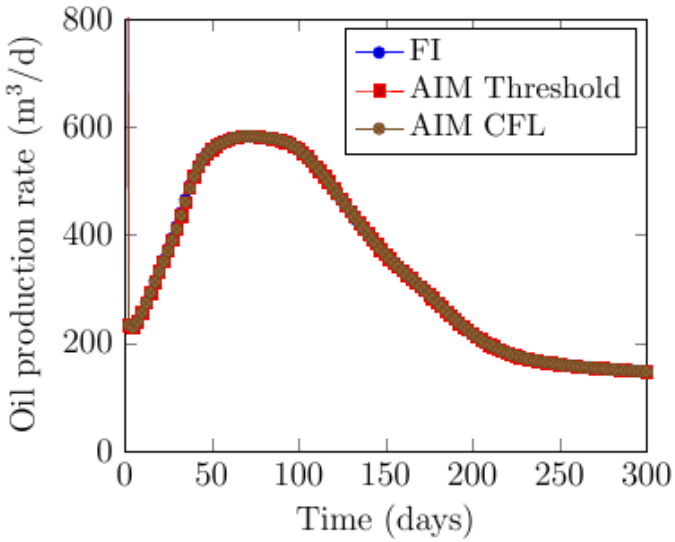

Figure 9. Oil production rates for Case 1

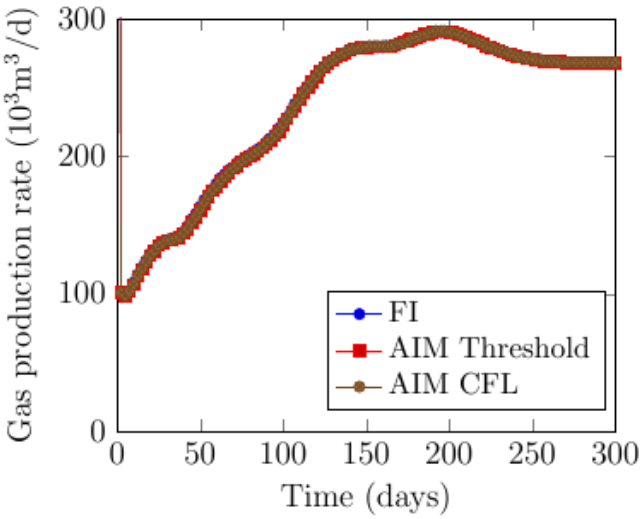

Figure 10. Gas production rates for Case 1

The production curves for the FI approach and the AIM approaches are in good agreement, indicating the AIM approach was correctly implemented. The threshold applied here was 0.01. Note that the results for the two adaptive approaches are presented in Figs. 9 and 10. They differ on the switching criterion adopted. The performance results are shown in Table 6.

Table 6. Simulation data comparison for Case study 1

Formulation	Avg. DT (d)	Step	FI%	CPU time (s)	Norm. time
IMPEC	-	-	-	FAILED	-
FI	0.005	-	100.0	274,477	1.00
AIM threshold	0.005	1500	0.011	152,444	0.55
AIM CFL	0.005	1500	11.32	163,031	0.59

From Table 6, we can observe that the AIM approach using both switching criteria greatly outperforms the FI simulation, while requiring a much smaller amount of FI blocks, as shown in the *FI%* column. Additionally, we should note that the *Step* parameter designates the number of time steps used to check the level of implicitness of the simulation.

4.2 Case 2: quarter of five-spot two-dimensional grid

The second case study is very alike the first one regarding the fluid data, reservoir data and operational conditions. The main differences lie in the reservoir shape, porosity, and permeability fields. We now have a quarter of five-spot configuration with two wells, one injector and one producer, in a grid composed of triangular and quadrilateral elements with a total of 7,942 grid nodes. Different from case study 1, we now have a homogenous absolute permeability and porosity fields.

Table 7. Reservoir data for Case study 2

Property	Value
Length, width and thickness	170.68 m, 170.68 m, 30.49 m
Porosity	0.35
Permeability (X and Y)	9.86×10^{-15} m², 9.86×10^{-15} m²

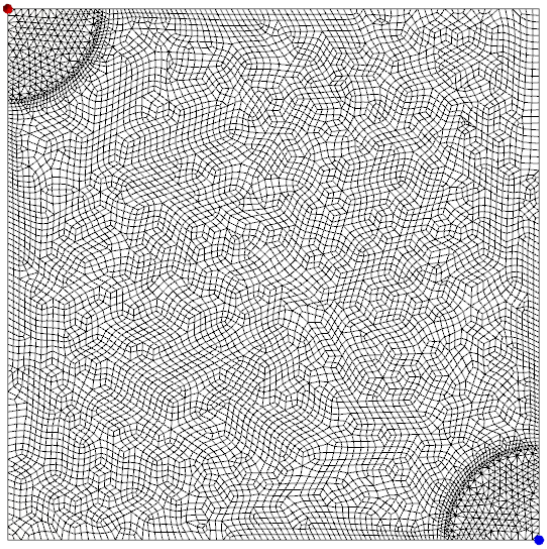

Figure 11. Hybrid grid with 7,942 gridblocks

Figures 12 and 13 present the oil and gas production for 2,000 days of production. Once again, we can observe that curves from the AIM approaches are in good agreement with the IMPEC and FI approaches. We can also verify that for this simpler case, the IMPEC simulation was correctly performed.

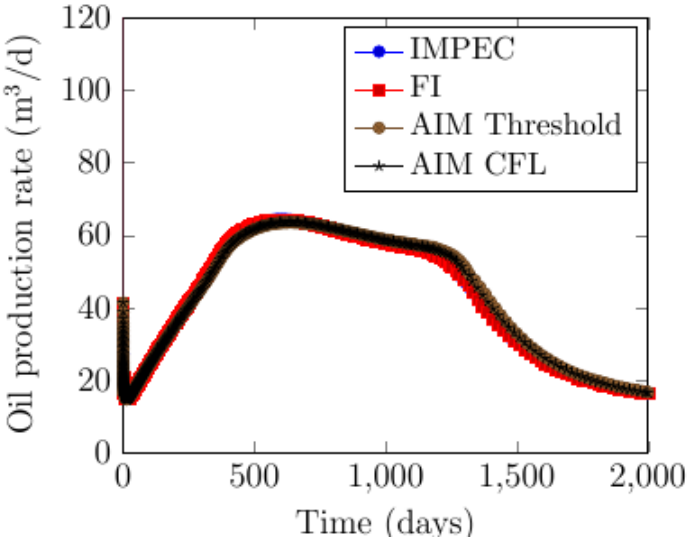

Figure 12. Oil production rates for Case 2

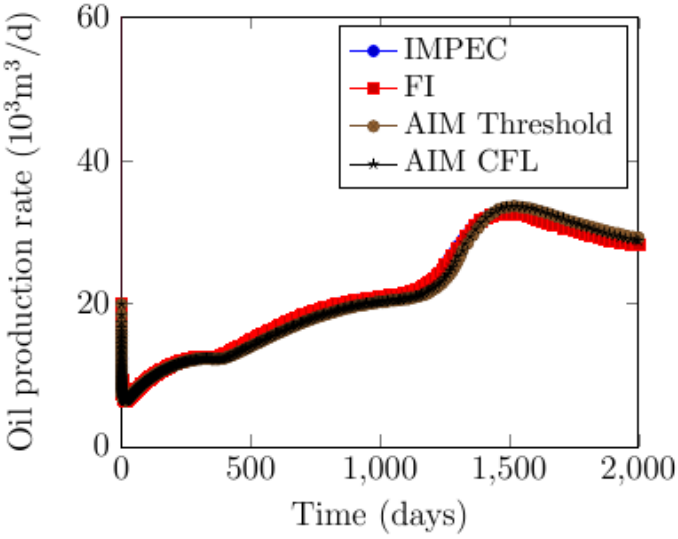

Figure 13. Gas production rates for Case 2

The CPU time performance is shown in Table 8. From this table, we can verify that the AIM approach was at least four times faster than the IMPEC and two times faster than the FI. The time step size for the adaptive method is comparable to the one used by the FI, while requiring much fewer implicit blocks. Also, the AIM based on the threshold required a very small percentage of FI gridblocks, compared to the AIM based on the CFL. The threshold was set to 0.1 for this case.

Table 8. Simulation data comparison for Case 2

Formulation	Avg. DT (d)	Step	FI%	CPU time (s)	Norm. time
IMPEC	0.019	-	0.00	19,131	1.00
FI	0.282	-	100.0	9,012	0.47
AIM threshold	0.274	200	0.074	4,053	0.21
AIM CFL	0.276	200	22.27	4,623	0.24

5 SUMMARY AND CONCLUSIONS

In the present work, we have implemented an AIM approach for two-dimensional compositional reservoir simulation in conjunction with unstructured grids and the EbFVM approach. Two switching criteria to change the gridblocks from IMPEC to FI and vice-versa were also implemented and tested: the threshold and the CFL criteria. From this investigation

some conclusions can be drawn. First, the Adaptive Implicit Method has shown, at least for the tested two-dimensional grids, that is able to reproduce the same results as of IMPEC and FI simulations; it is important to stress that both formulations from UTCOMPRS have been completely tested using commercial and in-house simulators. Second, the AIM formulation presented a significant improvement in performance up to nearly five times faster than IMPEC and twice faster than FI simulations.

From the results presented, the AIM approach has a great potential to replace the FI and IMPEC formulations. Additionally, combining this methodology with the EbFVM and unstructured grids allows for the simulation of real field applications.

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