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ON THE NUMERICAL RESERVOIR SIMULATION OF SINGLE PHASE TWO COMPONENTS FLOW ALONG WITH INTERMEDIATE TIME STEPS

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Abstract. *The goal of this work is to develop a numerical reservoir simulator to study an isothermal single-phase two-components porous media flow, and we use different time steps as a strategy for reducing computational time. The Peng-Robinson equation of state is used along with a volume translation to evaluate fluid properties. To solve the partial differential equations, we use a discrete grid and the Finite Difference Method, with a time implicit formulation and a first-order upwind scheme. We also use an operator splitting technique, and the decoupled equations for the pressure and the molar fraction are solved using the Conjugate Gradient and Bi-conjugated Gradient Stabilized methods. Therefore, the pressure equation is solved just once while the molar fraction equation a couple of times for a full-time step. The results show that the use of intermediate time steps may result in decreased computational effort.*

Keywords: *compositional flow, equation of state, finite difference method, reservoir simulation*

1. INTRODUCTION

Porous media flow is a research area with many applications in engineering, including contamination and water transport (Li and Yin, 2017), carbon sequestration (Das and Dutta, 2017), and hydrocarbons recovery (Zaydullin *et al.*, 2014; Wu and Sun, 2016). Considering the last example, we see that reservoir simulation is important and it is applied to assist the management of oil and gas resources (Chen, 2007).

Two models are most common when dealing with reservoir simulation: black-oil and compositional. We use the black-oil model to study conventional recovery when the fluid properties are a function of pressure (Young and Stephenson, 1983). On the other hand, we employ compositional models when changes in composition cause changes in the fluid flow inside the reservoir (Ertekin *et al.*, 2001).

Studying the compositional model usually requires an equation of state (EOS) (Amooie and Moortgat, 2018) to evaluate the physical properties of the components. Here, we used the Peng-Robinson EOS, with a volume translation, which is a very common equation of state applied in reservoir simulation (Chen and Chen, 2012).

To solve our compositional model, we considered the Finite Differences Method, which is very common in numerical reservoir simulation problems (Chen, 2007), with an upwind scheme (Versteeg and Malalasekera, 2007). This method leads to a system of equations, which are separated into two subsystems to be solved sequentially, one for the pressure and other for the molar fraction.

Solving the two subsystems means that we can use different methods to find the solution of the subsystems for the pressure and the molar fraction. So, we used the Conjugate Gradient Method to solve the pressure subsystem and the Bi-Conjugate Gradient Method for the molar fraction subsystem since we implement the coefficient matrices in a different way (Chen *et al.*, 2006; Debossam *et al.*, 2019).

As we used two different approaches, we are also able to take different time steps when solving each subsystem (Douglas *et al.*, 2000). This is a strategy to enhance the computational efficiency of our simulator. So, we increase the time step size (for a particular subsystem) to reduce the total number of iterations.

2. GOVERNING EQUATIONS

In this work, we are interested in numerical simulation of an isothermal single-phase two components flow considering advection and dispersion effects. We obtain the governing partial differential equations from the continuity equation, Darcy's law, and rock and fluid properties (Chen, 2007). Thus, we have for the phase

$$\frac{\partial}{\partial t}(\phi\xi) = \nabla \cdot \left[\frac{\xi}{\mu}\mathbf{k}\left(\nabla p - \gamma \nabla z\right)\right] + q, \tag{1}$$

where p is the pressure, ϕ is the porosity, ξ is the molar density, μ is the fluid viscosity, $\mathbf{k}$ is the absolute rock permeability tensor, γ is the product of density and gravity magnitude, z is the depth and q a source term. Considering chemical components,

$$\frac{\partial}{\partial t}(\phi x_m \xi) = \nabla \cdot \left[\frac{x_m \xi}{\mu}\mathbf{k}\left(\nabla p - \gamma \nabla z\right) + \phi\xi\mathbf{D}_m \nabla x_m\right] + q_m \qquad m = 1, 2, \ldots, N_c, \tag{2}$$

where x_m is the molar fraction, $\mathbf{D}_m$ is the dispersion tensor (Chen, 2007), q_m is a source term and N_c is the number of components.

For the evaluation of fluid properties, we use the Peng-Robinson equation of state (PR-EoS) with a volume translation (Wu and Sun, 2016). The molar density is a function of the compressibility factor, Z, such as

$$\xi = \frac{p}{RTZ}, \tag{3}$$

where R is the universal gas constant, and the Peng-Robinson cubic equation can be written as

$$Z^3 - (1 - B)\,Z^2 + \left(A - 2B - 3B^2\right) Z - \left(AB - B^2 - B^3\right) = 0, \tag{4}$$

where A and B are parameters that are functions of critical temperature and pressure such as

$$A = \frac{ap}{R^2T^2}, \tag{5}$$

$$B = \frac{bp}{RT}, \tag{6}$$

where a and b are the mixture rule parameters (Peng and Robinson, 1976).

As Eq. (4) has three roots, only real roots are selected. We take the largest root for gas flow, whereas we choose the smallest positive root for oil flow (Wu and Sun, 2016).

Some parameters of the EoS are specific for vapor pressure. Thus, a volume translation must be used to avoid errors when using the equation of state for liquids (Chen, 2007),

$$v_{corr} = v_{EoS} + C, \tag{7}$$

where the volume v is the reciprocal of the molar density ξ, and C is the correction factor, and it is computed using temperature and component's properties (Hoyos, 2004).

Due to the reservoir heterogeneous nature and non-linearities, like the pressure dependence for the fluid properties, we must solve Eqs. (1) and (2) numerically for the pressure and molar fraction, respectively.

3. METHODOLOGY

We solve the partial differential equations using the finite difference method, which is widely applied in reservoir simulation problems (Ertekin *et al.*, 2001; Chen, 2007). We also use an implicit time formulation, a first-order upwind scheme, and an operator splitting technique (Vennemo, 2016) along with a linearization that allows solving pressure and molar fraction equations as separate subsystems. Therefore, as already mentioned, we use different time steps when solving these two subsystems.

We obtain the pressure subsystem by applying the finite difference method to Eq. (1) (we neglect gravity):

$$\left[V_b c\left(p^{n+1}\right)\frac{p^{n+1} - p^n}{\Delta t}\right]_{i,j,k} = \sum_{l \in \psi_r}\left[T_{l,r}^{n+1}\left(p_l^{n+1} - p_r^{n+1}\right)\right] + q_{i,j,k}^{n+1}, \tag{8}$$

where $r = i, j, k$, ψ_r is the neighbor nodes, $V_b = L_xL_yL_z$, $A_x = L_yL_z$, $A_y = L_xL_y$ and $A_z = L_xL_y$. The transmissibility T is defined by

$$T_{x,i\pm\frac{1}{2},j,k}^{n+1} = \left(\frac{\xi k_{xx} A_x}{\mu \Delta x}\right)_{i\pm\frac{1}{2},j,k}^{n+1}. \tag{9}$$

and for y- and z-directions analogous equations can be written. The $c(p)$ function is the compressibility, defined as

$$c(p) = \phi \frac{\partial \xi}{\partial p} + \xi \frac{d\phi}{dp} \tag{10}$$

where porosity ϕ is considered as a function of pressure only.

For the molar fraction subsystem, Eq. (2), we employ a similar approach:

$$\left[V \frac{(\phi x_m \xi)^{n+1} - (\phi x_m \xi)^n}{\Delta t} \right]_r = \sum_{l \in \psi_r} \left[(x_m T)^{n+1}_{l,r} \left(p^{n+1}_l - p^{n+1}_r \right) \right] + \sum_{l \in \psi_r} \left[\mathcal{D}^{n+1}_{m,l,r} \left(x^{n+1}_{m,l} - x^{n+1}_{m,r} \right) \right] + q_m, \tag{11}$$

where $\mathcal{D}_m$ is given by (Chen, 2007)

$$\mathcal{D}^{n+1}_{m,i+\frac{1}{2},j,k} = \phi \xi D_m \frac{A_x}{\Delta x}, \tag{12}$$

for x-direction, and analogous expressions for y- and z-directions. We use an upwind scheme to determine the molar fractions x_m, which we evaluate at the interfaces of the cells ($x \pm 1/2$, for example).

In the numerical procedure we solve first Eq. (8), for pressure, and then Eq. (11), for molar fraction, in all cells. This is a Sequential Implicit Method (operator splitting) since we solve implicitly both pressure and molar fraction (Kou and Sun, 2004; Maes *et al.*, 2016). Again, as the system is solved separately, the time step used for each "sub-problem" may be different.

Therefore, we introduced an intermediate time step (Abreu, 2007). In theory, this strategy can reduce the computational cost, since it modifies the frequency in which we solve the two equations. In general, at each full-time step, we solve the two equations only once when we consider the same time step for both equations. However, with the introduction of an intermediate time step, the molar fraction equation can be solved a couple of times while solving the pressure equation only once, allowing to use a larger time step for the pressure equation while maintaining a smaller time step for the molar fraction.

To obtain the pressure and molar fraction for each time step, we must solve the uncoupled linear subsystems. We perform this task by applying the Conjugate Gradient Method to solve the pressure equation (symmetric coefficient matrix) and the Bi-conjugated Gradient Stabilized Method for the molar fraction equation (asymmetric coefficient matrix) (Saad, 2003).

We adopt the more challenging problem of fluid flow through a Naturally Fractured Reservoir (NFR), as an example of an application, to highlight the potential of the strategy. In this case, we must consider two different regions: matrix and fracture (or fracture network). In general, fractures have greater permeabilities and porosities than the porous matrix (Nelson, 2001).

4. NUMERICAL RESULTS

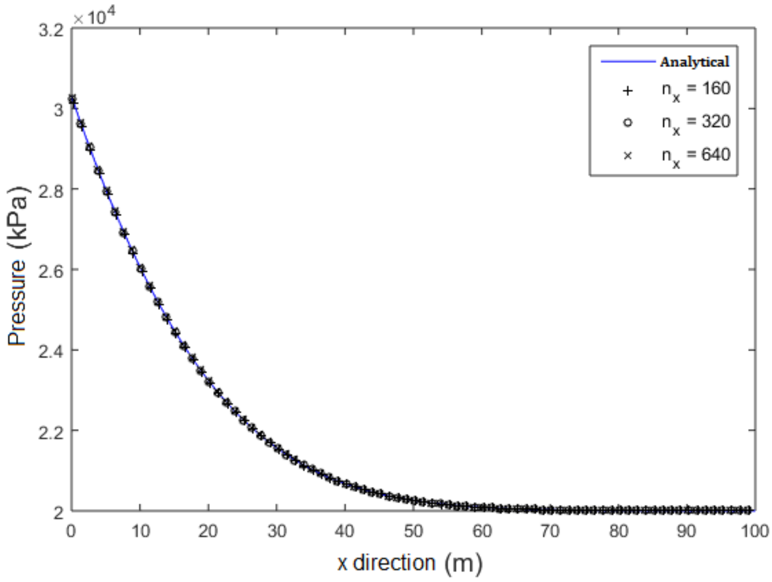
We obtained the numerical results considering a compositional flow in a three-dimensional reservoir imposing a prescribed pressure in both west and east sides, while there is no mass flux through the other boundaries. In the west boundary, a heavier component is flowing into the reservoir. We used a Dell PowerEdge R720 with Intel Xeon E5-2620 processor to perform all simulations.

To verify our code, we used two known analytical solutions: one for the pressure (Rosa *et al.*, 2006) and another for the molar fraction (Lake, 1989). They are valid for simplified one-dimensional problems with constant coefficients. We can find more details under what conditions they are valid in Debossam (2018). In Figure 1, we can see that our results are in good agreement with the analytical solution and that the number of cells n_x, in the x-direction, has no influence on the accuracy.

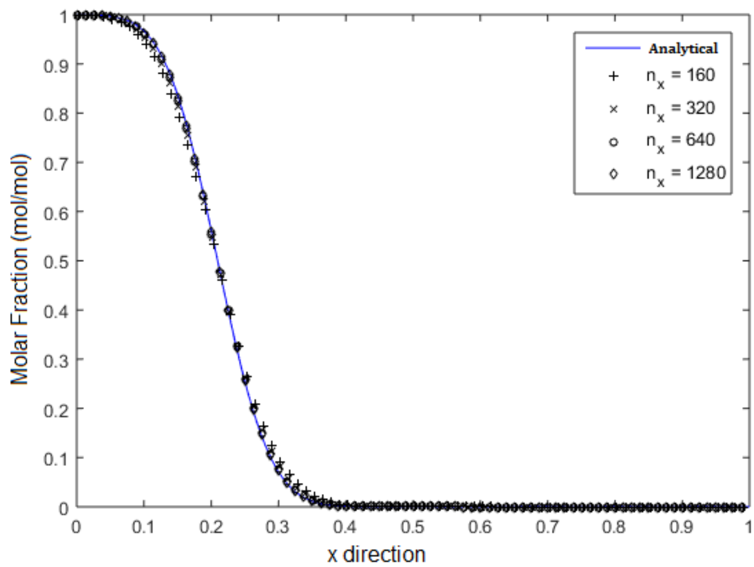
4.1 Reservoir without fractures

For the first simulations, the reservoir does not contain fractures and the time step for the molar fraction (Δt_c) is kept constant and equal to 0.5 days, while the time step for the pressure (Δt_p) assumes the values 1, 5, 10, 20 and 40 times Δt_c.

Figure 2 shows that keeping the same value for Δt_c while increasing Δt_p didn't result in an observable change in the behavior of the molar fraction field. When the Number of Intermediate Steps (NIS) is equal to one, we have the default case where the time steps used to solve pressure and molar faction equations are the same. Only when $\Delta t_p = 40\Delta t_c$, we can see a significant variation in the results for the molar fraction. However, we think that this difference is due to the use of a large time step for the pressure system, which leads to a larger truncation error and this error is propagated to the molar fraction field. When we calculate the pressure using intermediate time steps, for this particular problem, the results contain little to no difference.



(a) Pressure



(b) Molar fraction

Figure 1: Comparison between analytical and numerical solution for pressure and molar fraction

In Table 1 we have a comparison between the NIS and the Total Simulation Time (TST). What we note is that there is a significant gain in performance using the intermediate time steps and that it attains a maximum value at about NIS equal to 20, showing that with a NIS bigger than this we start to lose efficiency and accuracy.

Table 1: Time of simulation for the first test.

NIS	TST	Time Variation
1	4h:22min:29s	–
2	3h:21min:35s	-23.20%
5	2h:25min:22s	-44.62%
10	2h:07min:48s	-51.31%
20	1h:59min:11s	-54.59%
40	2h:10min:16s	-50.37%

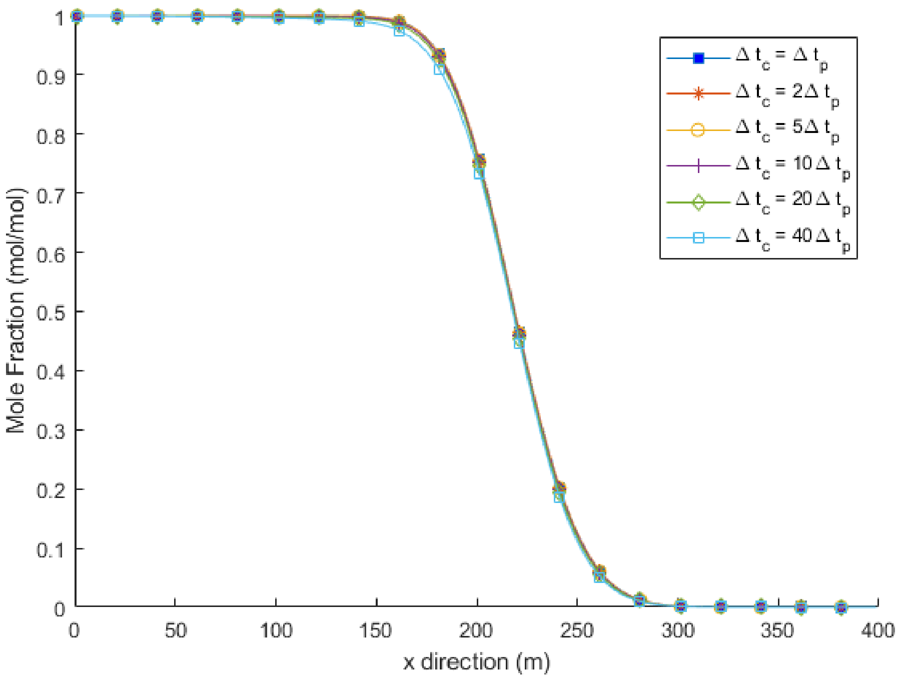


Figure 2: Molar fraction for the first test for different time steps ratio

4.2 Naturally fractured reservoir

We performed another test with a naturally fractured reservoir containing four fractures, equally spaced and positioned in the same abscissa. Refer to Table 2 for fracture length (l_x) and location (x_0, y_0) in the xy-plane. The porosity of the matrix is ϕ_m=0.2, while the fractures have ϕ_f=0.6. The permeability for the matrix is k_m=20 mD and for the fractures k_f=50$\times$10^3 mD, or 2,500 times greater than that of the porous matrix.

Table 2: Location and properties of fractures

Parameter	Fracture 1	Fracture 2	Fracture 3	Fracture 4
l_x (m)	200	200	200	200
x_0 (m)	50	50	50	50
y_0 (m)	25	75	125	175

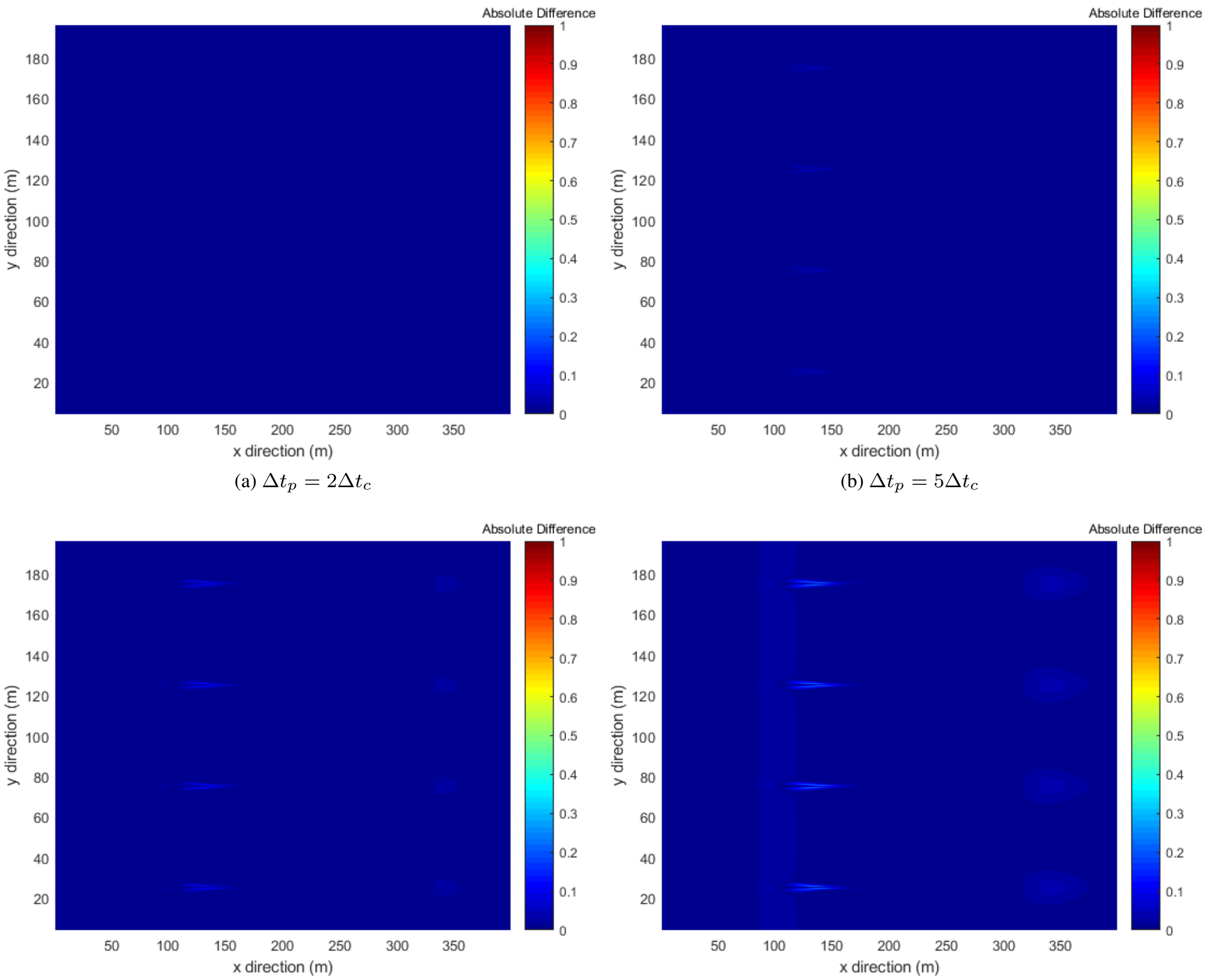
As before, Fig. 3 shows a comparison between the results obtained with and without the use of an intermediate time step. The figure contains a plot of the absolute difference between the molar faction values determined using a Δt_p 2, 5, 10, and 20 times greater than Δt_c. As we can observe, the difference is not significant, mainly for a NIS equal to 2 or 5, when the difference is barely noticeable. However, for the 10:1 and 20:1 ratio we notice, near the fractures, that the difference is not negligible, mostly when we are considering 20 intermediate steps. This tendency is also found when we have a 40:1 ratio, meaning that the absolute difference becomes even greater. Again, the pressure results almost do not change when using the intermediate time steps.

Table 3 is the one corresponding to Table 1 for the flow in the fractured reservoir. For the case in question, we remark that the execution time reaches a maximum reduction with ten intermediate time steps. However, we have an increase in the absolute difference error for the molar fraction. Nevertheless, when we use a 5:1 (or even 10:1) time step ratio, we achieve a reduction of approximately thirty percent of CPU time. Even so, the results still show a small error, making it an appropriate choice when seeking better performance accompanied by a little loss of accuracy.

In Figure 10, we have a comparison between the molar fraction fields when using only one and ten intermediate time steps, which was our most efficient simulation. Despite knowing that there are differences, as shown in Figure 2, in practice, it is difficult to perceive the difference between these fields.

Another test case was carried out with the fractures being positioned non uniformly in the reservoir. In this case, the four fractures have different lengths and properties. Table 4 shows the properties and positions of the fractures for this new arrangement, where l_x represents the length of the fracture and (x_0, y_0) the coordinates indicating the positioning of fractures in the xy-plane.

Figure 5 shows, as in the previous case, a comparison between the molar fraction fields for this specific simulation. Once again, we only used a NIS equal to 1 and 10, and we realize that there is no noticeable difference.



(a) $\Delta t_p = 2\Delta t_c$ (b) $\Delta t_p = 5\Delta t_c$

(c) $\Delta t_p = 10\Delta t_c$ (d) $\Delta t_p = 20\Delta t_c$

Figure 3: Absolute relative difference between the molar fraction values

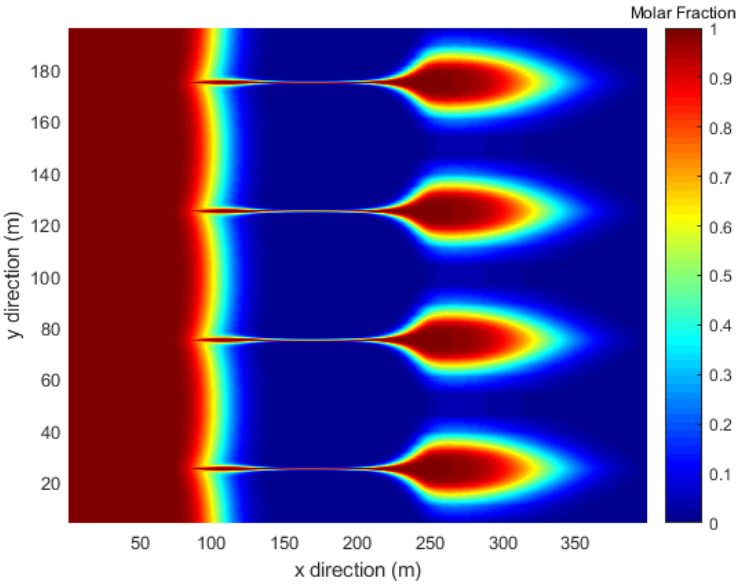
Table 3: Total simulation time for the second test.

NIS	TST	Time Variation
1	62h:38min:54s	–
2	61h:12min:26s	-2.30%
5	46h:19min:05s	-26.07%
10	43h:14min:46s	-30.97%
20	43h:54min:25s	-29.92%
40	56h:33min:51s	-9.71%

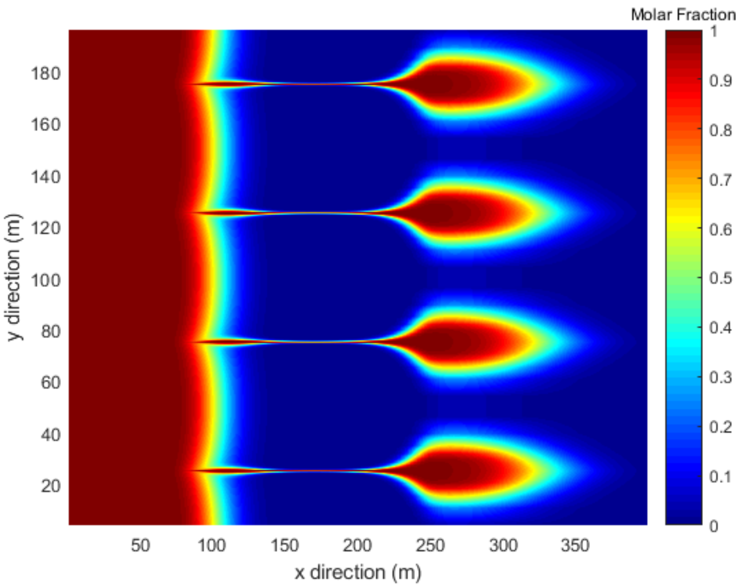
Table 4: Location and properties of fractures

Parameter	Fracture 1	Fracture 2	Fracture 3	Fracture 4
l_x (m)	100	70	120	200
x_0 (m)	30	180	80	40
y_0 (m)	35	135	85	175
k_f (D)	25	100	50	35
ϕ_f	0.5	0.8	0.6	0.6

As expected, for this more complex problem with sharp differences between fracture properties, the simulation times were longer than those of the uniform arrangement and fractures having the same permeability and porosity. For the



(a) $\Delta t_p = \Delta t_c$



(b) $\Delta t_p = 10\Delta t_c$

Figure 4: Molar fraction comparison without and with intermediate steps

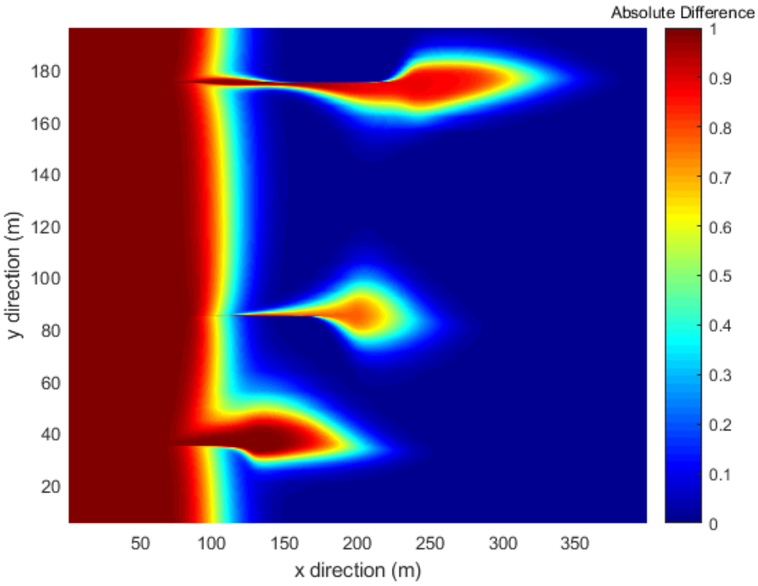
default case (NIS = 1), the simulation lasted 90 hours, 27 minutes, and 43 seconds. On the other hand, when we have a NIS = 10, the simulation ended after 39 hours, 52 minutes, and 39 seconds. This corresponds to a time reduction of 55.92%. Therefore, this indicates that the technique may be advantageous and that this approach can be used as an alternative in other scenarios when we want to reduce the simulation time.

5. CONCLUSION

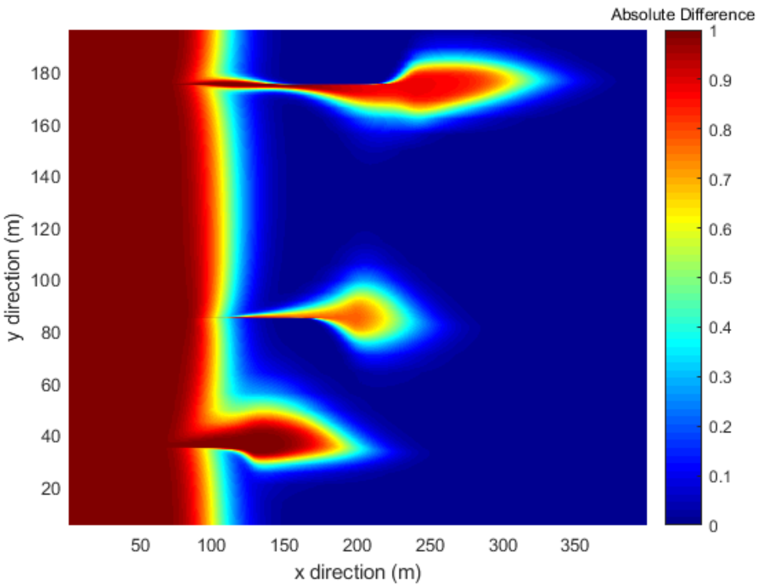
This work presented an alternative to speed up complex two components reservoir simulation when solving the uncoupled partial differential equations for pressure and molar fraction. The methodology enabled the introduction of intermediate time steps resulting in a significant reduction in execution time, despite the little loss of accuracy when we obtain the results without a time step partitioning technique.

Depending on the number of time steps employed, we can achieve different CPU time reductions. We obtained our best results for a NIS ranging between 10 and 20, showing that we can attain an optimal time reduction, but we left this discussion for future work.

Although the first results are encouraging, it is worth noting that this strategy was successful for our problem and particular test cases. Therefore, there is no guarantee that this strategy will work the same way for other problems and



(a) $\Delta t_p = \Delta t_c$



(b) $\Delta t_p = 10\Delta t_c$

Figure 5: Molar fraction for the new fracture arrangement

scenarios. Nevertheless, it is a potential tool that deserves additional studies to prove its efficiency and reach.

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8. RESPONSIBILITY NOTICE

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