A Modified Sequential Method for Solving the Full Composition Model in Numerical Reservoir Simulation

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Abstract. A modified sequential method (MSEQ) is proposed in this article to solve the full composition model in numerical reservoir simulation. During the iterative process, in order to solve the composition equations efficiently, the pressure field is treated as fixed temporarily, then the topological sorting algorithm is employed to update the saturation and mole friction field. Through the topological sorting for the grids from upstream to downstream, the full field coupled composition equations can be decoupled and solved with high efficiency as same as the explicit difference scheme. Numerical tests are performed and the high performance of the proposed MSEQ is illustrated. It can predict the simulation results with the same accuracy, and its computational speed is more than 2 times faster than the fully implicit method (FI) and the traditional sequential method (TSEQ).

1. Introduction

CO2 flooding has become an important way to exploit low permeability reservoir [1]. In order to accurately simulate the complex process of CO2 displacement, a full composition model is usually used. At present, the numerical methods of solving the full component model mainly include three kinds of methods: the fully implicit method (FI), the implicit-pressure explicit-saturation/concentration algorithm (IMPESC), and the sequential solution algorithm (SEQ). The efficiency of IMPESC method within a single time step is very high, but its stability is poor because of the use of explicit saturation and composition, which requires a enough small time step [2]. Thus, it cannot be applied to the engineering applications. Coats [3] used a fully implicit method to solve the composition equations. Though FI is of high numerical stability, its efficiency is extremely low due to its direct solving for all the coupled unknown variables. As an alternative way, SEQ method can reduce the memory usage and improve the calculation efficiency. In the traditional SEQ method, all the coupled component equations are still solved simultaneously even though the pressure field is treated as known.

In fact, the component equations are hyperbolic and the convection term should be discretized in upwind scheme to ensure the numerical stability. For a single hyperbolic equation, scholars have proposed a topological sorting algorithm [4-7]. The topological sorting algorithm is employed in this article to solve composition equations. Though topological sorting of the grids from upstream to downstream, the discrete composition equations can be decoupled and solved independently within their own grids.
This paper is organized as follow. In the section 2, the mathematical model is introduced. The topological sorting algorithm in sequential method is described in the section 3. Numerical tests are provided in the section 4, and conclusions are drawn in the section 5.

2. Mathematical model
If neglecting the CO2's dissolution in the water and the capillary pressure, the material balance for the water and \(cN\) hydrocarbon compositions yields the following \(N_c+1\) different equations in the full composition model for isothermal CO2 flooding:

\[
\frac{\partial}{\partial t} (\phi \rho_w S_w) = \nabla \cdot \left( \frac{K_{nw}}{\mu_w} \rho_w \nabla P \right) + wq_w, \tag{1}
\]

\[
\frac{\partial}{\partial t} \left[ \phi (\rho_w S_w + \rho_o S_o) z_i \right] = \nabla \cdot \left( \frac{K_{no}}{\mu_o} \rho_o x_i \nabla P \right) + \nabla \left( \frac{K_{no}}{\mu_o} \rho_o y_i \nabla P \right) + q_i. \quad (i = 1, 2, \cdots, N_c) \tag{2}
\]

Where \(\phi\) is porosity; the subscripts \(w, o, g\) represent water, oil and gas phase respectively; \(\rho\) is molar density of the \(\alpha\) phase; \(S\) is phase saturation; \(K\) is permeability; \(\mu\) is viscosity; \(P\) is pressure; \(q\) is molar injection/production rate of water; \(x\) and \(y\) are the mole fraction of component \(i\) in oil and gas phase respectively; \(q_i\) [8] is molar injection/production rate of component \(i\).

The total molar fraction \(z\) can be determined by

\[z_i = Lx_i + (1-L)y_i, \tag{3}\]

With \(L = \frac{\rho_o S_o}{\rho_o S_o + \rho_w S_w}\).

The additional constraint equations are needed for solving (1), (2) and (3).

The saturation constraint is

\[S_w + S_o + S_g = 1.0. \tag{4}\]

The two mol fraction constraints for \(x\) and \(y\) are:

\[\sum_{i=1}^{N} x_i = 1.0. \tag{5}\]

\[\sum_{i=1}^{N} y_i = 1.0. \tag{6}\]

The fugacity constraints express the requirement that liquid and vapor phase fugacities must be equal for each component:

\[f_i^L = f_i^V, \quad (i = 1, 2, \cdots, N_c). \tag{7}\]

The above total \(3N_c + 4\) equations correspond to the \(3N_c + 4\) unknowns \(x, y, z, p, S_w, S_o, S_g\). Details of calculating the fugacity \(f^L, f^V\) can be referred to SRK equation of state [9]. The other parameters such
as the molar density $\rho_x$, relative permeability $K$ and viscosity $\mu$ can all be seemed as the functions of the above $3N + 4$ unknowns.

3. Topological sorting algorithm in sequential method

Generally speaking, solving the above equations simultaneously requires lots of computer memory since the number of hydrocarbon compositions maybe quite large. Thus, the direct fully implicit method is hard to be applied for some cases in the practical engineering. The sequential method is one of the alternative ways to realize the numerical simulation of full composition model by combining the sequential solving and iteration process.

3.1. Sequential solving of the full composition model

In sequential method, the $l$th iteration in each time step of solving the full composition model equations (1)-(7) is divided into three steps.

First, fix $z^{i-l}$ at its existing iterative value, then solve the total pressure equation (8) and (3) with their constraints (4)-(7) to update the $l$th iterative value of the pressure, saturation and mol fraction (denoted as $1_{1l}P$, $1_{1l}S$, $1_{1l}x$, and $1_{1l}y$). The total pressure equation can be obtained by adding all the (1) and (2):

$$\frac{\partial}{\partial t} \left[ \phi \left( \rho_x S + \rho_S S_x + \rho_u S_u \right) \right] = \nabla \cdot \left( \rho_x \frac{K_S}{\mu_x} \nabla P \right)$$

$$\nabla \cdot \left( \rho_S \frac{K_S}{\mu_S} \nabla P \right) + \nabla \cdot \left( \rho_u \frac{K_u}{\mu_u} \nabla P \right) + \sum_{i=1}^{N} q_i.$$ (8)

Second, fix $P^{i-l}$ and $z^{i-l}$ at their existing iterative values, then solve (3) with their constraints (4)-(7) to update the $l$th iterative value of the saturation and mol fraction (denoted as $2_{1l}S$, $2_{1l}x$, and $2_{1l}y$). The cost of this step is ignorable since solving of (1) or (2) is avoided in this step and the unknown variables can be solved independently in their own blocks.

Third, fix $P^{i-l}$ at its existing iterative values, then solve the composition mass conservation equations (2) and (3) with their constraints (4)-(7) to update the $l$th iterative values of the saturation and mole fraction (denoted as $3_{1l}S$, $3_{1l}x$, $3_{1l}y$, and $3_{1l}z$). Till now, all the unknown variables are updated to their $l$th iterative values $1_{1l}, 1_{1l}P, 1_{1l}S, 1_{1l}x, 1_{1l}y$.

It needs to be mentioned that the second step is optional. Implementing of this step will strengthen the convergence of the algorithm.

3.2. Topological sorting algorithm for composition equation

When solving the composition mass conservation equations (2), the upwind scheme is always used. The interface parameters such as

$$(\rho_{1l}K_{1l}x_{1l}/\mu_1)^{i-l}_{i_{1l}+1/2, i_{1l}+1}, (\rho_{1l}K_{1l}x_{1l}/\mu_1)^{i-l}_{i_{1l}+1/2, i_{1l}+1}, (\rho_{1l}K_{1l}x_{1l}/\mu_1)^{i-l}_{i_{1l}+1/2, i_{1l}+1}, (\rho_{1l}K_{1l}y_{1l}/\mu_1)^{i-l}_{i_{1l}+1/2, i_{1l}+1}, (\rho_{1l}K_{1l}y_{1l}/\mu_1)^{i-l}_{i_{1l}+1/2, i_{1l}+1}, (\rho_{1l}K_{1l}z_{1l}/\mu_1)^{i-l}_{i_{1l}+1/2, i_{1l}+1},$$

take their values from the upstream grid. It means that the discrete node equation only involves the variables in the local and upstream grids. If the pressure field has been calculated out, the upstream grid can be prescribed. Under this situation, solving the node equations according to their topological order (from upstream to downstream) can reach the high efficiency as same as the explicit difference scheme.

In the step 3 mentioned above, since the pressure field is not updated in this step, the grids can be sorted from upstream to downstream. After sorting, the total unknown variables can be correspondingly expressed as $(u, u, \cdots, u)$ with $u_i = \left( z^{i-l}_{i_{1l}}, x^{i-l}_{i_{1l}}, y^{i-l}_{i_{1l}}, z^{i-l}_{i_{1l}} \right)$ and $N$ being the total number of the grids.

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Notice that $u_{k+1}$ is always at the downstream of $u_k$, so the nodal equation for $u_k$ do not contain the items relevant to $u_m (m > k)$. That is, the node equations can also be sorted and expressed as

\begin{align*}
F_1(u_1) &= 0, \\
F_2(u_1, u_2) &= 0, \\
&\cdots \\
F_i(u_1, u_2, \cdots, u_k) &= 0, \\
&\cdots \\
F_N(u_1, u_2, \cdots, u_N) &= 0.
\end{align*}

These equations are solved one by one according the above order. When solving the nodal equation $F_i(u_1, u_2, \cdots, u_k) = 0$ for $u_k$, actually all the other variables $u_1, u_2, \cdots, u_{k-1}$ have been solved out already. Thus, this equation $F_i(u_1, u_2, \cdots, u_k) = 0$ can be solved directly. Through this way, the coupled equations (9) are decoupled and can be solved with high efficiency as same as the explicit difference scheme.

4. Numerical examples

In this chapter, two examples are provided to illustrate the computational efficiency of the proposed modified sequential method (MSEQ). For simplicity, only the one-dimensional case is tested though the proposed algorithm is also suitable for high dimensional cases. The simulation area is 128m long. For comparison, the simulation results from the fully implicit scheme (FI) and traditional sequential solution method (TSEQ) are also provided. Gaussian elimination method is employed to solve the linear algebraic equations for all the three methods.

In both examples, CO2 is injected from the left boundary and the cross-sectional area is supposed to be 1m². We set initial pressure $P=14.0E+6$Pa, injection pressure $P_i=16.0E+6$Pa, temperature $T=350$K, $\Delta t=500$s, porosity $\varphi=0.35$, permeability $k=1.0$md and relative permeability $k_r=S^2$.

4.1. Example 1

In this example, three compositions are contained. The initial distribution of the three compositions is shown in Table 1. The number of grids is 128.

| Composition | Total Mole Fraction |
|-------------|---------------------|
| CO2         | 0.0                 |
| C1          | 0.03767             |
| C22         | 0.96233             |

Fig. 1 shows the variation of the cumulative oil production with time calculated from the three schemes, and Fig. 2 shows the distribution of gas phase saturation at $t=10^6$ day. It can be seen that the simulation results from the proposed MSEQ is as accurate as the FI and TSEQ. The total CPU time used for MSEQ is 180.1s in this example, while for the FI and the TSEQ, the total CPU time is 406.9s and 457.7s respectively. It means that the proposed MSEQ is more than twice as efficient as the FI and the TSEQ.
4.2. Example 2
In the second example, nine compositions are contained, which makes the simulation more complicated. The initial distribution of the nine compositions is shown in Table 2.

Table 2. The initial mole fractions of the nine compositions in Example 2

| components | Molar Fraction |
|------------|----------------|
| CO₂        | 0.0032         |
| N₂         | 0.0322         |
| C₁         | 0.2687         |
| C₂         | 0.108          |
| C₃         | 0.0772         |
| C₄         | 0.0537         |
| C₅         | 0.0384         |
| C₆         | 0.0367         |
| C₇+        | 0.3819         |

Three quality grids are employed with their numbers being 128, 256 and 512 respectively. The simulation results of the 128 grids are shown in Fig. 3 and 4 at t=10th day. The accuracy of the proposed
MSEQ is confirmed. It can predict the same cumulative oil production and saturation distribution as the FI and TSEQ. The total CPU times used for the three schemes under different quality grids are shown in Table 3. It can be seen that the proposed MSEQ is still more than twice as efficient as the FI and the TSEQ even in this complicated example. The high efficiency performance is maintained for all the different grids employed in this example.

![Image](image1)

**Figure 3.** Variation of the cumulative oil production with time in Example 2

![Image](image2)

**Figure 4.** The distribution of gas phase saturation at $t=10^{th}$ days in Example 2

| Grid Number | MSEQ         | TSEQ         | FI          |
|-------------|--------------|--------------|-------------|
| 128         | 300.6875     | 760.4688     | 941.4688    |
| 256         | 696.9375     | 1412.266     | 1780.969    |
| 512         | 1192.109     | 2533.844     | 3313.688    |

**Table 3.** The total CPU times (s) used in Example 2 for the three schemes under different quality grids

5. Conclusion
In this article, a modified sequential method (MSEQ) is proposed to solve the full composition in numerical reservoir simulation. When solving the composition equations during the iterative process, we fix the pressure field temporarily, then the topological sorting algorithm can be employed to update the saturation and mole friction field. Through the topological sorting for the grids from upstream to downstream, the full field coupled composition equations can be decoupled and solved with high efficiency.
efficiency as same as the explicit difference scheme. Numerical tests show that the proposed MSEQ can predict the simulation results with the same accuracy, and its computational speed is more than 2 times faster than the fully implicit method (FI) and the traditional sequential method (TSEQ).

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