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Fully Implicit Mixed Hybrid Finite-Element Formulation for General-Purpose Compositional Reservoir Simulation

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Abstract

We present a fully implicit mixed hybrid finite-element (FE) formulation for general-purpose compositional reservoir simulation. The formulation is locally conservative, and the momentum and mass balance equations are solved simultaneously; including Lagrange multipliers on element interfaces. The method utilizes automatic differentiation for the Jacobian construction. This hybrid FE approach accommodates unstructured grids, and we present black-oil and compositional test cases with permeability tensors. We also discuss the accuracy and computational efficiency for the new formulation. For all tests, we compare the performance and accuracy of the proposed approach with the Multi-Point Flux Approximation (MPFA-O) method.

Introduction

The mixed finite element (MFE) finite-element method solves for the mass and momentum balance equations simultaneously (Chavent & Jaffre, 1986; Berzzi & Fortin, 1991; Abushaikha, et al., 2015). The method is locally conservative, and it can accommodate high-order elements and anisotropic material properties. However, in its original form, MFE leads to an algebraic system of saddle-point type whereby the linearized matrix is indefinite. An efficient variant for the method was developed to overcome this issue: where Lagrange multipliers, for the primary variables, are appended on the elements interfaces (Chavent & Roberts, 1991). This approach is called the mixed hybrid finite element (MHFE) method, and we present a fully implicit version of MHFE in this paper. Another approach to overcome the saddle point problem is to eliminate the momentum balance equation from the linear system, and replace it with a multi-point flux approximation in the mass balance, see (Wheeler & Yotov, 2006) for more details. This elimination procedure can be considered a special case for the MPFA-O method (Matringe, et al., 2007; Younes, et al., 2010; Aavatsmark, 2002). We apply the MPFA-O method in the comparison study in this paper.

Previous MHFE-based efforts include (Younes & Fontaine, 2008); Chavent et al. (1990) used the method for modeling two-phase incompressible fluids; Hoteit & Firoozabadi (2006) extended the method for compositional equation-of-state models, and gravity was included by Moortgat & Firoozabadi (2016).

However, all the schemes were designed for specific problems and have not been applied for general-purpose reservoir simulation.

In this work, we employ the MHFE method for general-purpose compositional reservoir simulation fully implicit in time. The velocities are of high order and approximated with Raviart-Thomas vector basis functions (Raviart & Thomas, 1977). The scalar variables (pressure, fluid and component concentrations) are discretized using discontinuous Garelkin's method. We employ the fully implicit scheme whereby the conservation equations are coupled and the system is linearized using Newton-Raphson method. The non-linear variables are spatially discretized on the elements and on the element's interfaces by the hybridization process. The MHFE method is implemented in the Automatic Differentiation General Purpose Research Simulator (AD-GPRS) (Voskov & Tchelepi, 2012; Zaydullin, et al., 2014; Garipov, et al., 2016; Younis, et al., 2011; Zhou, 2012).

To validate the proposed approach, we perform a numerical analysis highlighting the convergence and accuracy for the method. We also compare the discretization to MPFA-O. Moreover, we apply the method for reservoir simulation problems, with the emphasis on unstructured domains and tensor permeability, to illustrate its application and robustness for general-purpose reservoir simulation.

The paper is organized as follows. In Section 2, the governing equations are discussed. In Section 3, the mixed hybrid finite element is described, and in Section 4, the nonlinear solution is detailed. We validate the method using challenging cases with convergence studies in Section 5 and 6. Finally, in Section 7, we present our conclusions.

Governing equations

We consider isothermal multi-component compositional flow model for a three-phase (oil, water and gas) system, namely,

$$\frac{\partial}{\partial t}\left(\phi \sum_{\alpha} x_{c\alpha}\rho_{\alpha}S_{\alpha}\right) + \nabla \sum_{\alpha} x_{c\alpha}\rho_{\alpha}u_{\alpha} = \sum_{\alpha} x_{c\alpha}\rho_{\alpha}q_{\alpha}\,, \qquad c = 1, \ldots, n_c$$

The Darcy law for phase α reads as:

$$u_{\alpha} \quad = \quad -(\mathbf{k}\frac{k_{r\alpha}}{\mu_{\alpha}}(\nabla p_{\alpha} - \gamma_{\alpha}\nabla D)), \alpha = o, w, g$$

where ϕ is the porosity of the medium, $x_{c\alpha}$ is the concentration of component c in phase α, ρ_{α} is the phase molar density, S_{α} is phase saturation, u_{α} is Darcy velocity of phase, q_{α} is source of phase, $\mathbf{k}$ is the intrinsic permeability tensor, μ_{α} is dynamic phase viscosity, p_{α} is phase pressure, $\gamma_{\alpha} = \rho_{\alpha}g$ is vertical pressure gradient, D is vertical depth vector (downward oriented), $k_{r\alpha}$ is phase relative permeability and computed in this paper by

$$k_{r\alpha} = k^{o}_{r\alpha}S^{o^{n_{\alpha}}}_{\alpha}, S^{o}_{\alpha} = \frac{S_{\alpha} - S_{\alpha i}}{1 - S_{\alpha i} - S_{\alpha' r}}$$

Where n_{α} is Corey parameter, $k^{o}_{r\alpha}$ is the end-point relative permeability, S^{o}_{α} is the normalized phase saturation, $S_{\alpha i}$ is initial phase saturation and $S_{\alpha' r}$ is residual saturation for the other phase.

For the three-phase multi-component system, we assume instantaneous thermodynamic equilibrium between the hydrocarbon liquid and vapor phases (Zaydullin, et al., 2012). In addition, the hydrocarbon components do not dissolve in the water phase, and the water component exists in the water-phase only. The thermodynamic equilibrium is described by the following equations:

$$f_{cg}(p,T,x_{cg}) - f_{co}(p,T,x_{co}) = 0, \qquad c \in [1,\dots n_h]$$

$$z_c - V x_{cg} - L x_{co} = 0, \qquad c \in [1,\dots n_h]$$

$$L + V - 1 = 0,$$

$$\sum_{c=1}^{n_h} (x_{co} - x_{cg}) = 0.$$

Where

$$V = \nu_g/(1-\nu_w), L = \nu_o/(1-\nu_w), z_c = Z_c/(1-\nu_w).$$

where $f_{c\alpha}$ is the fugacity, z_c is overall mole fractions of component c, and $n_h = n_c - 1$. We assume that p, T and z_c are known. Next, we define $x_{c\alpha}$ and ν_α. For compositional simulation, the following procedures are applied to define the phase behavior:

- The phase stability test - for the current p, T and z_c, - we find the phase state (liquid, vapor or two-phase) of the composition. This test is needed for any element whose status at the previous Newton iteration is single-phase.
- The flash calculation – we apply it if the phase stability test indicates that the phase state of the element changed from single to two phases, therefore we solve the system in order to obtain the x_{co}, x_{cg}, and $V(L)$. Note the vapor-liquid distribution ratio, K-value=x_{cg}/x_{co}, from the stability analysis can be used as an initial guess.

In this paper, the phase stability test and flash calculations are based on the standard approach described in (Michelsen, 1982; Michelsen, 1982). Here, we use the Compositional Space Adaptive Tabulation (CSAT) approach (Voskov & Tchelepi, 2009; Voskov & Tchelepi, 2009).

In order to close the system of conservation equations, additional relations are required. These relations are introduced as local equations (based on the unknowns in the element) and include different types of physical constraints. In this work, the constraints are:

$$\begin{aligned} \sum_{c=1}^{n_c} x_{c\alpha} - 1 &= 0, \quad \forall \alpha = o, g \\ \sum_{\alpha=o,w,g} S_\alpha - 1 &= 0, \\ p_\alpha &= p - p_{c,\alpha}, \quad \forall \alpha = w, g \end{aligned}$$

where p is the oil phase pressure and $p_{c,\alpha}$ is the capillary pressure.

The primary unknowns for the governing equations are based on the natural-variables formulation (Coats, 1980), and they are defined by the phase pressures, $p_{c,\alpha}$, phase saturations, S_α, and molar fractions of the components, $x_{c\alpha}$. Next, we describe the discretization method for this work.

Mixed hybrid finite element method

In this work, we use the MHFE method to discretize the conservation equations. The method estimates the fluxes at the interfaces of an element using vectorial basis functions where the flux is unity at interface and zero elsewhere.

$$\int_{A_j^E} \mathbf{W}_i^E \cdot \mathbf{n}_j^E = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

where $\mathbf{W}_i^E$ is the vectorial basis function of interface i, $\mathbf{n}_j^E$ is the normal outward oriented vector on interface j and A_j^E is the area of interface j of element E. Another property of the mixed formulation is that $\nabla \cdot \mathbf{W}_i^E$ is constant over an element,

$$\int_{V^E} \nabla \cdot \mathbf{W}_i^E = 1$$

where V^E is volume of element E. Since the vectorial basis functions are of a high order, we can estimate the velocity field anywhere in the element using the following equation

$$\mathbf{u}^E = \sum_{i=1}^{N_f} \mathbf{W}_i^E Q_i^E$$

Where $\mathbf{u}^E$ is the approximate solution of velocity vector in element E, Q_i^E is the flux at interface i of element E, N_f is the number of interfaces in element.

We refer the reader to (Abushaikha, et al., 2016) for the discrtritization details for the conservation equations. Next, we discuss the nonlinear solution of the primary variables.

Nonlinear solution

We discuss the procedure for the nonlinear solution for the unknowns. We use the Newton-Raphson method to linearize the system, in which a Jacobian system is assembled and solved for each nonlinear iteration for our fully-implicit system:

$$\begin{bmatrix} J_{PP} & J_{P\lambda} \\ J_{\lambda P} & J_{\lambda\lambda} \end{bmatrix} \begin{bmatrix} \partial y_P \\ \partial y_\lambda \end{bmatrix} = \begin{bmatrix} R_P \\ R_\lambda \end{bmatrix}, \qquad p,\ S_\alpha,\ x_{c,\alpha} \in y_P, \qquad \lambda_p,\ \lambda_{c,\alpha} \in y_\lambda$$

Here, R_P is residual for the thermodynamic equilibrium and the mass balance equations discussed in Section 2; R_λ is the residual for the momentum balance for advection and capillarity (Abushaikha, et al., 2016); J is the derivative for the element and interface variables, and it is automatically assembled and analytically derived using our Automatic Differentiation Expression Templates Library (ADETL) (Younis, et al., 2011; Zhou, 2012) ; y are the primary unknowns (nonlinear variables).

The total set of nonlinear variables consist of:

- p, pressure
- S_α, phase saturation
- $x_{c,\alpha}$, phase composition of each component
- λ_p, pressure at element interface
- $\lambda_{c,\alpha}$, phase capillary pressure at element interface

This nonlinear formulations is an extension of the natural-variables formulation implemented in AD-GPRS for compositional systems with an arbitrary number of phases (Voskov, 2011). Here, we extend it by accounting for the Lagrange multipliers for the mixed hybrid finite element method.

For every nonlinear iteration, we define the number of co-existing phases in each element, and we compute an overall composition for each component:

$$z_c = \frac{\sum_\alpha x_{c\alpha} S_\alpha \rho_\alpha}{\sum_\alpha S_\alpha \rho_\alpha}$$

Then, we use the multiphase flash described in Section 2 to define the number of co-existing phases. Once the number of phases is determined, we update the unknowns S_α and $x_{c,\alpha}$ and systematically activate the corresponding governing equations in the Jacobian; whether for one-phase or two-phases. Finally, the linear system is solved for each Newton update:

$$\mathbf{J}(y^k)(y^{k+1} - y^k) + \mathbf{r}(y^k) = 0,$$

where k is the nonlinear iteration number. For this fully-implicit approach, we use a non-linear solver with Appleyard chopping (Wang & Tchelepi, 2013) with tolerance of 10^{-6}, and the linear solver in this paper is PARDISO 5.0 (Kuzmin, et al., 2013).

The numerical convergence

In this test, we consider a single-phase problem with exact pressure solution (Lipnikov, et al., 2006):

$$P^{ex}(x, y, z) = x^2 y^3 z + 3x\sin(yz)$$

The domain is a uniform cube $[0,1]^3$ with Dirichlet boundary condition on the boundaries. The full permeability tensor is distributed in the domain by:

$$K(x, y, z) = \begin{bmatrix} y^2 + z^2 + 1 & xy & xz \\ xy & x^2 + z^2 + 1 & yz \\ xz & yz & x^2 + y^2 + 1 \end{bmatrix}$$

We validate the discretization of the MHFE method for this problem by comparing the reference solution to the numerical solution and computing the discretization error. In Figure 1, we show the error for the numerical solutions for the MHFE and the MPFA-O schemes. The MHFE method producers less error than the MPFA-O scheme. The convergence rate for the MHFE is quadratic.

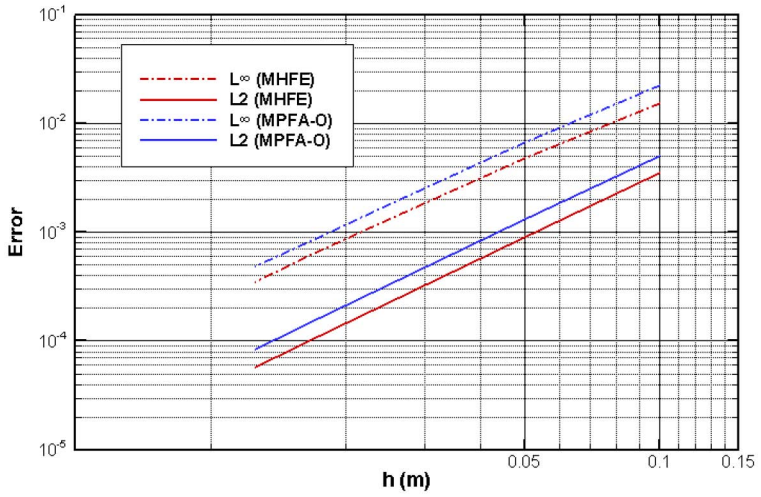

Figure 1—Error for MHFE and MPFA-O schemes. The MHFE method models the single-phase with full tensor peremability more accurately than the MPPFA-O scheme. h is the element size.

Top layer of SPE10 with permeability tensor

In this section, we present a challenging heterogeneous case for the SPE10 (Christie, et al., 2001) with tensorial permeability that follows the stratigraphy of an unstructured domain (see Figure 2): the global

direction of the permeability is rotated to follow the direction of the stratigraphy of the domain. We test for black-oil and compositional equation of state models. The mesh is composed of 87,996 tetrahedron elements, and we compare the MHFE method to the MPFA-O method. As a measure of time-step size, we use the component-based CFL criteria which is defined as:

$$CFL_c = \frac{\Delta t}{V\phi} \frac{\sum_\alpha \rho_\alpha Q_\alpha x_{c,\alpha}}{\sum_\alpha \rho_\alpha S_\alpha x_{c,\alpha}}$$

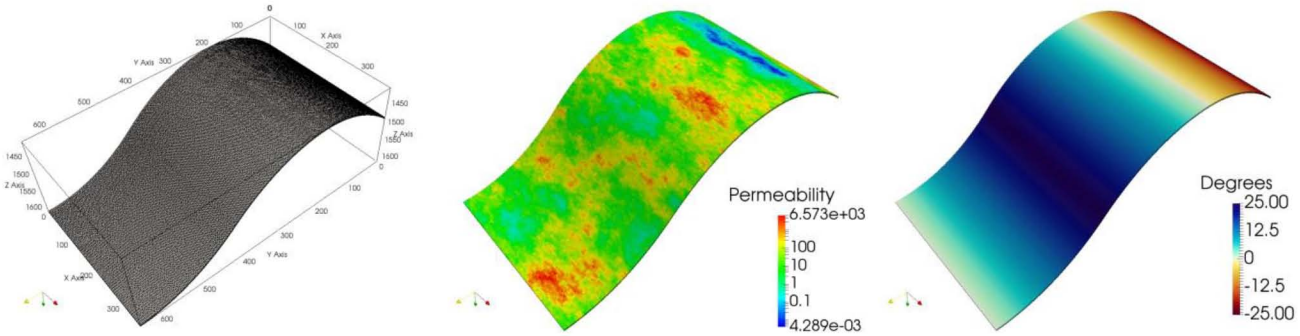

Figure 2—Top layer of SPE 10 in an unstructured domain. mesh (left), permeability (center), and angle of stratigraphy (right).

The scenarios for the permeability distribution for the domain are:

$$K = \begin{cases} \text{diag}\left(k, k, \frac{k}{10}\right), & \text{for scenario M1} \\ R_y(-\theta)\text{diag}\left(k, k, \frac{k}{10}\right) R_y(\theta), & \text{for scenario M2} \end{cases}$$

Where $R_y(-\theta)$ is the rotation matrix by θ about the y axis using the right-hand rule, and θ is stratigraphic angle of the domain and varies from 25 to -25, as shown in Figure 2.

Black oil case

In this case, we introduce four production wells at the corners of the domain and one injector at the top of the structure. The producers BHP is 200 Bar and the injector is 400 bar. The fluids properties are shown in Table 1. The capillary pressure is show in Figure A-1. We produce for 5000 days. Figure 3, shows the pressure, total velocity, and water saturation after 3000 days for M1 and M2. We can see the water propagating faster, while the pressure is less diffusive, for M2 thanks to the stratigraphical permeability tensor.

Table 1—Black oil case properties.

	z_{oil}	z_{gas}	Bubble point [bar]	R_s	B_o	B_g	μ_o [cp]	μ_w [cp]	ρ_o [kg/m^3]	ρ_w [kg/m^3]
Value	0.9348	0.0652	170	346.8	1.46	7.20E-03	0.412	0.318	859.5	1033

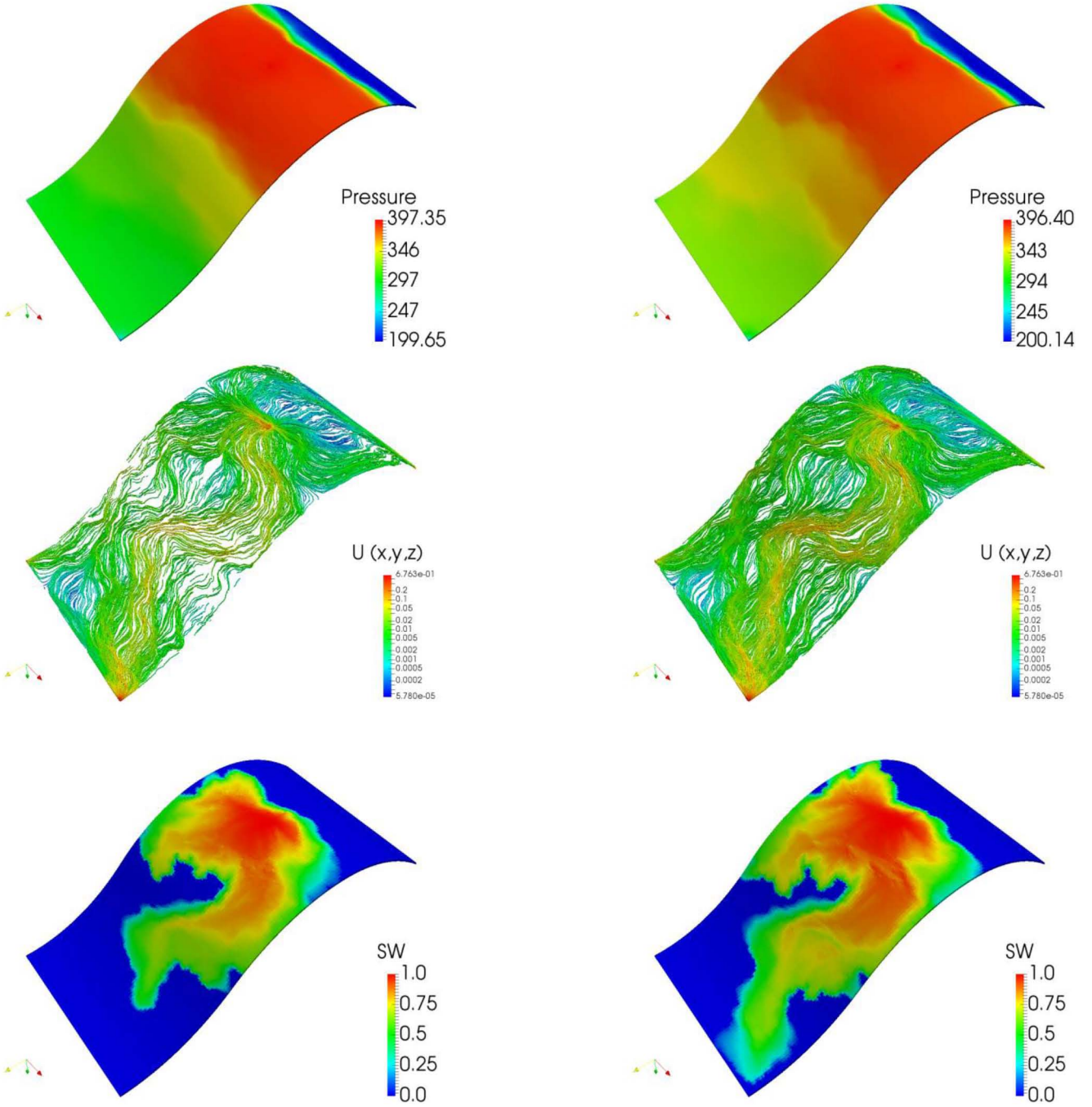

Figure 3—Pressure (bar), total velocity (m/day), and water saturation for the black oil case after 3000 days of production for scenarios M1 (left) and M2 (right).

We compare the MHFE method to the MPFA-O in Table 2 and Figure 4. The water breakthrough is faster for the MPFA-O scheme than MHFE since MPFA-O models a more diffusive pressure distribution as we saw in the convergence study. It is also computationally more expensive than MHFE since the MPFA-O has more stencils per flux. The MHFE models the solution more accurately than the MPFA-O thanks to the Lagrange multipliers appended on the elements interfaces. In Figure 5, we compare the water saturation difference between the cases. Next, we test the same domain for EoS model.

Table 2—Black oil case simulation results.

	Number of Steps		Non-Linear Iterations		CFL average		Water Breakthrough (days)		Normalized CPU time	
	M1	M2	M1	M2	M1	M2	M1	M2	M1	M2
MHFE	541	545	2452	2486	50.028	66.519	4040	3070	1.00	1.02
MPFA-O	542	542	2558	2567	53.746	72.839	3840	2860	1.41	1.45

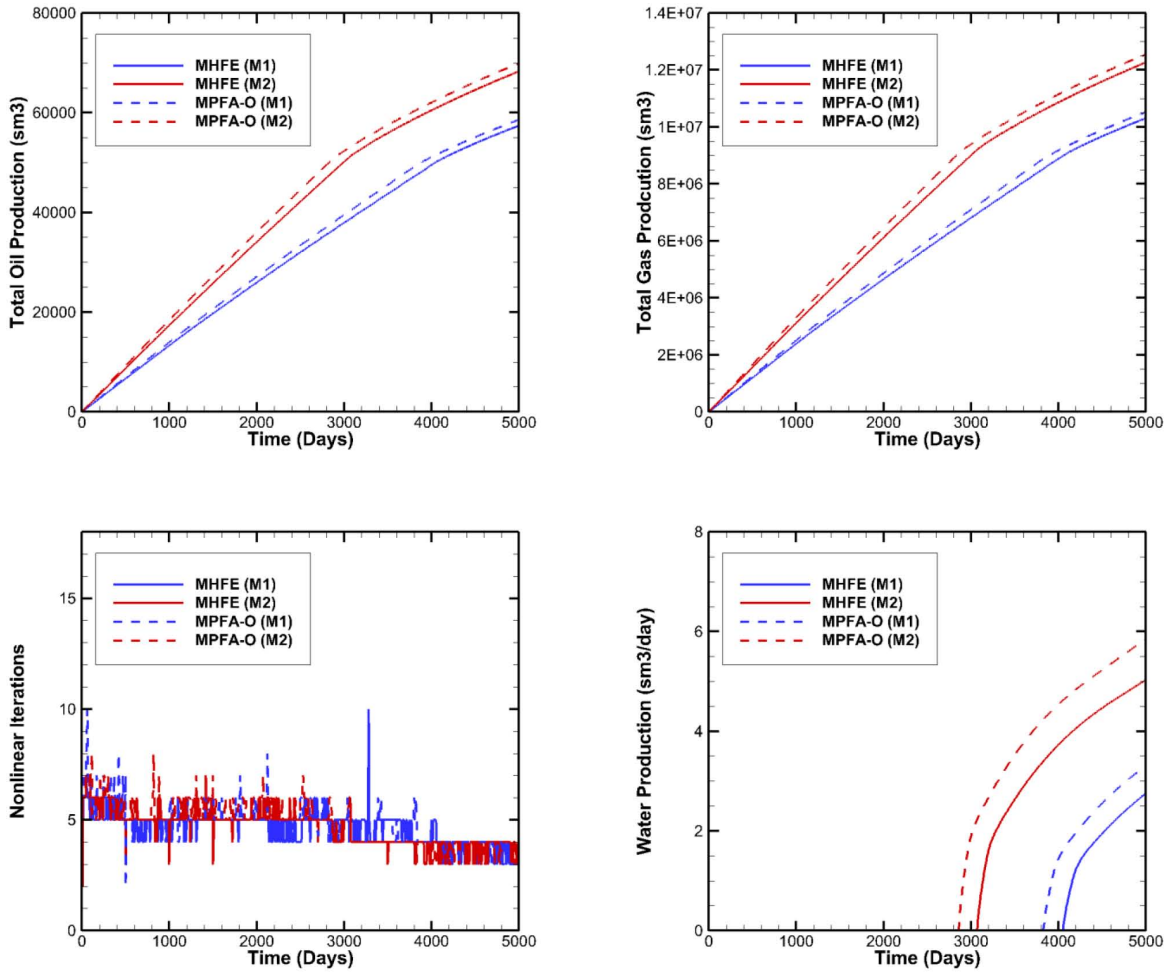

Figure 4—Black oil case simulation results for MHFE and MPFA-O.

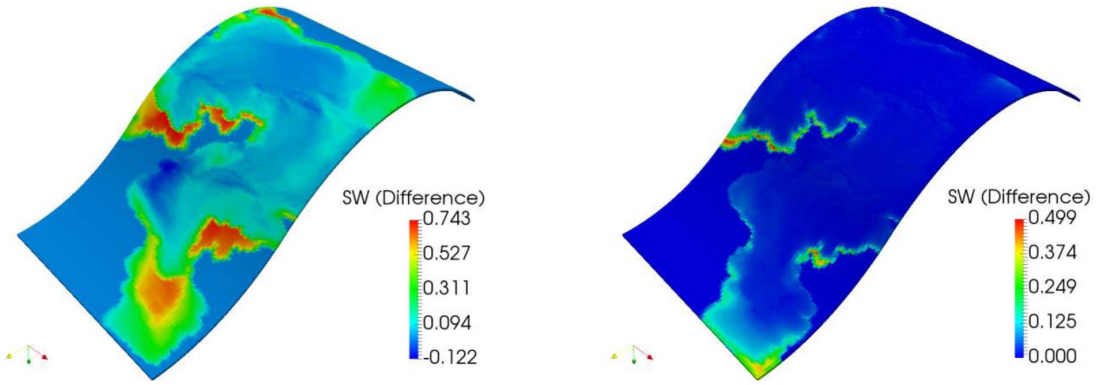

Figure 5—Black oil case water saturation difference after 3000 days of production between M2 and M1 for MHFE (left) and between MPFA-O and MHFE for M2 (right).

Compositional EoS case

In this case, the oil is comprised of four components; Co_2, CH_4, C_4 and C_{10}, see Table 3, and we introduce four production wells at the corners of the domain. The producers BHP is 140 Bar and we produce for 360 days. Figure 6 shows the pressure, total velocity after 250 days for M1 and M2. Figure 7 shows the production results for the M1 and M2. The production kinetics for scenario M2 is faster than M1 thanks to the stratigraphical permeability tensor. Moreover, the MPFA-O scheme has faster kinetics than the MHFE which is in agreement with the previous test: since the pressure is more diffusive for MPFA-O scheme. Again, the MPFA-O is computationally more expensive than the MHFA, as shown in Table 4, since the Jacobian stencils are larger and sparser than MHFE.

Table 3—Compositional case properties

	Z	Mol. Wt.	P_{crc} (bar)	T_{crc} (K)	V_{crc} (cm3/mol)	ω
CO2	0.01	44.010	73.86	304.2	92.64	0.2280
CH4	0.2	16.043	46	190.6	99.85	0.008
C4	0.29	58.124	38	425.2	254.99	0.193
C10	0.5	142.286	22.08	615.0	430.42	0.491

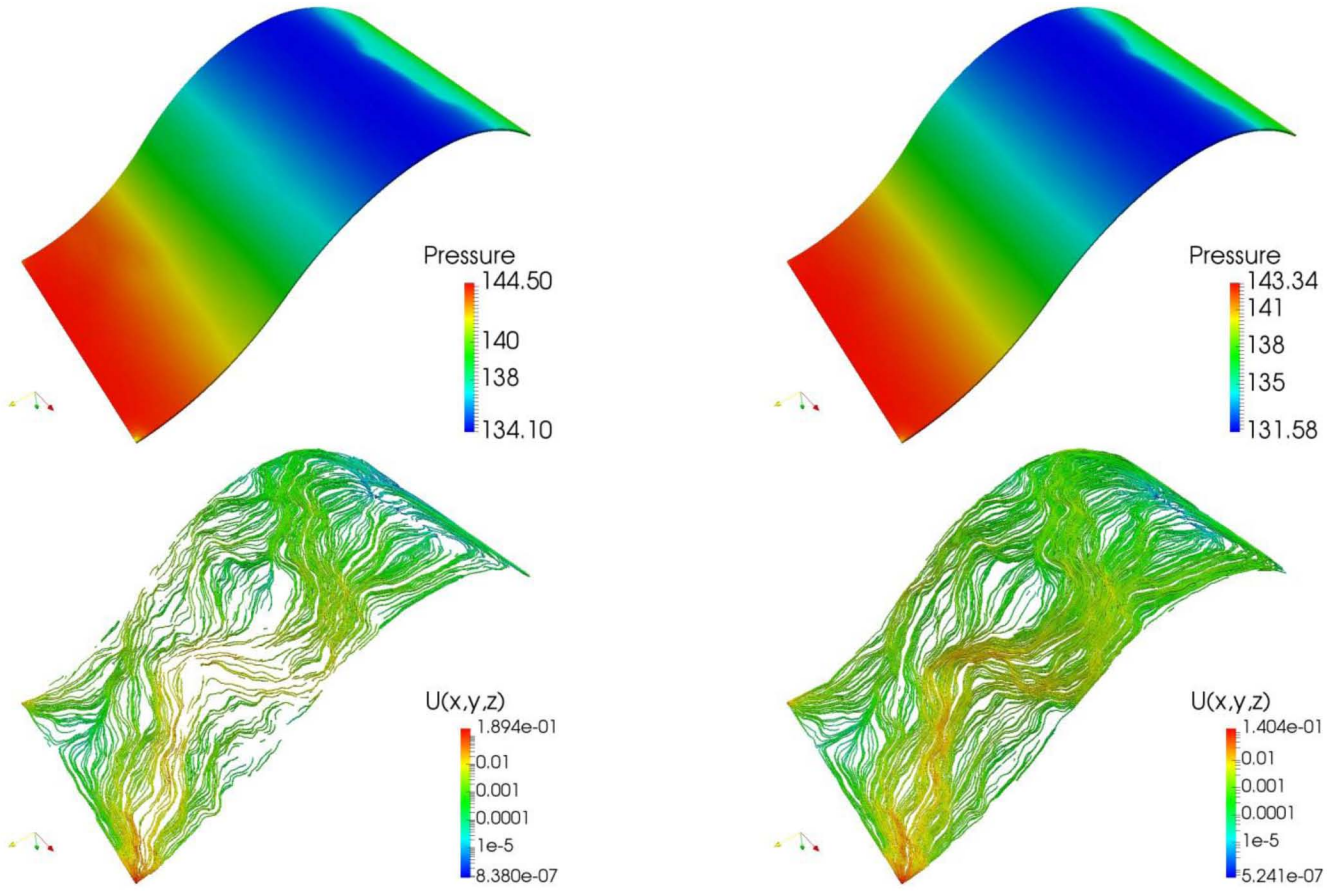

Figure 6—Pressure (bar) and total velocity (m/day) for the compositional case after 250 days of production for scenarios M1 (left) and M2 (right).

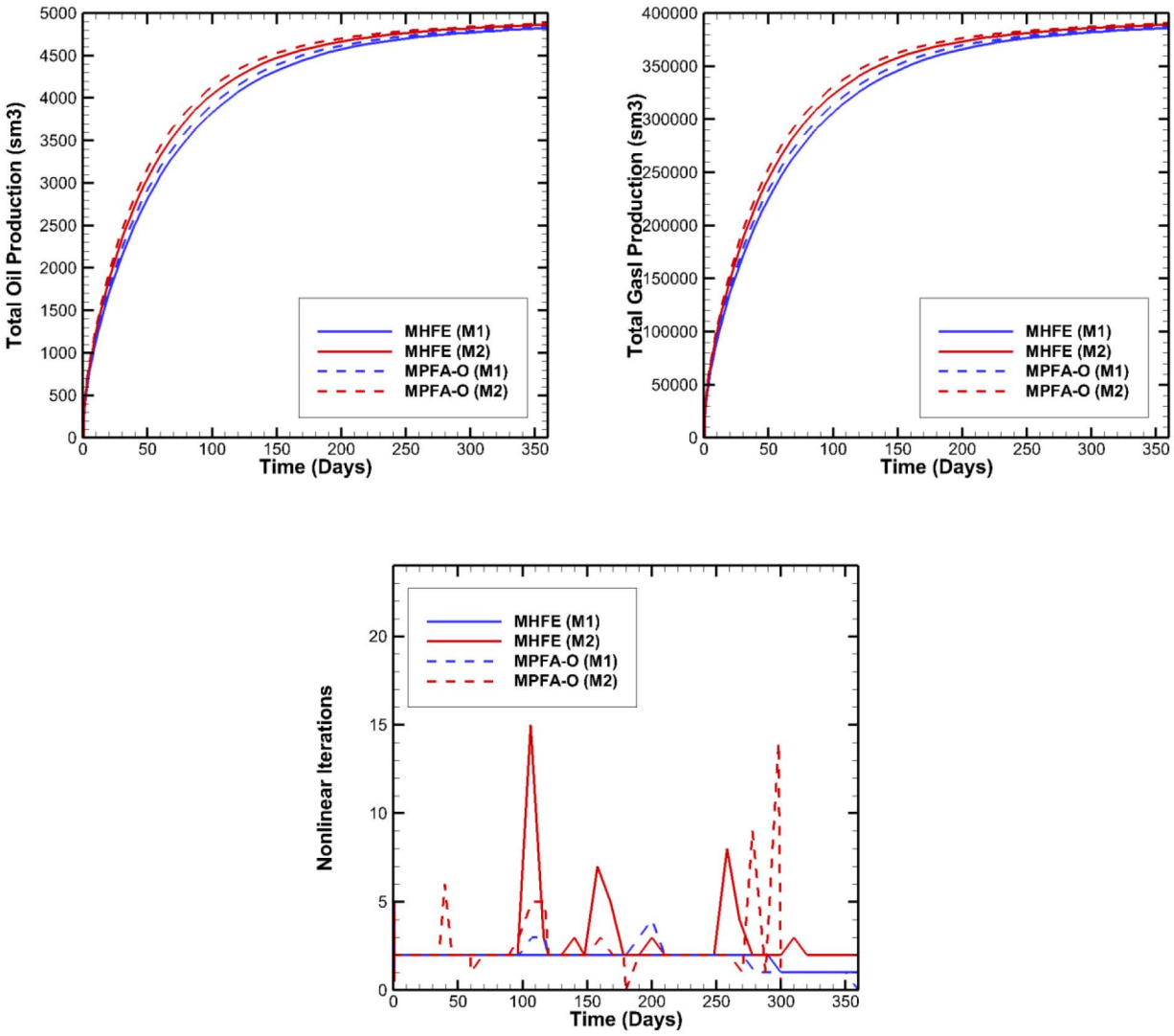

Figure 7—Compositional case simulation results for MHFE and MPFA-O.

Table 4—Compositional case simulation results

	Number of Steps		Non-Linear Iterations		CFL average		Normalized CPU time	
	M1	M2	M1	M2	M1	M2	M1	M2
MHFE	81	84	155	196	30.743	28.976	1.00	1.49
MPFA-O	81	86	156	183	31.068	28.764	1.50	2.31

Conclusion

In this paper, we presented a fully implicit mixed hybrid finite element method for general purpose compositional reservoir simulation. The proposed approach is numerically more accurate than the MPFA-O scheme. We presented black-oil and compositional Eos cases for unstructured domains with permeability tensors. The MHFE models the cases more accurately and efficiently than the MPFA-O, thanks to the hybridization approach of the mixed finite element where Lagrange multipliers are appended on the elements interfaces.

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Appendix

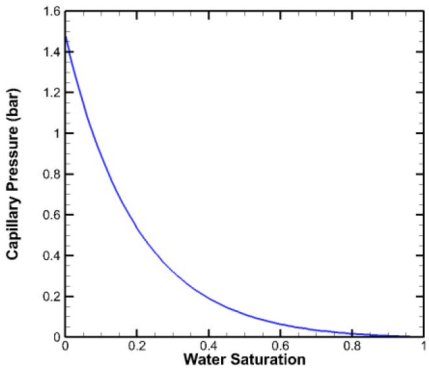

Figure A-1—Capillary pressure for Black-oil case.