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An OpenFOAM-based multiphase solver for physical systems with stationary and moving phases using a coupled solution for phase fractions

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Abstract. This work presents the formulation, verification, and application of an OpenFOAM-based multiphase solver for physical systems with moving and stationary phases. The latter is used to model porous media, allowing for the simulation of multiphase flow processes applied to many areas of science and engineering. The model considers an implicit coupled solution of the phase-fraction equations for an arbitrary number of phases in the system, providing better approximations when compared to the standard segregated solution. We present verification tests simulated in scenarios with different numbers of moving phases, along with an application case.

Keywords. OpenFOAM, Multiphase Flows, Porous Media, Coupled Solution

1 Introduction

Understanding the multiphase flow processes that occur in porous media, such as oil and gas reservoirs, is essential for managing these resources. Thus, the development of numerical tools to simulate productivity is a topic of interest to academia and industry [1]. In this context, open-source simulators are especially attractive due to the accessibility they offer to the scientific community. Here, we consider the OpenFOAM platform for CFD (Computational Fluid Dynamics) simulations. OpenFOAM is a powerful CFD software that employs the Finite Volume Method (FVM) to discretize and solve the governing equations of fluid flow and related phenomena. It offers a versatile platform in C++ for simulating and analyzing complex fluid dynamics problems, allowing users to accurately model and understand various physical phenomena through the integration of advanced numerical methods and customizable solvers [9].

There are several solvers for multiphase flow problems available in the OpenFOAM framework. One example is `multiphaseEulerFoam` [10], a solver based on the Eulerian multi-fluid model which considers averaged conservation equations. Another solver to be highlighted is `porousMultiphaseFoam` [4], a dedicated toolbox for incompressible two-phase flows in porous media. Furthermore, we recently developed `upstreamFoam` [6], a solver that combines the Eulerian multi-fluid formulation for a system of an arbitrary number of phase fractions for flows in

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porous media. It considers physical systems containing moving and stationary phases, and has a distinguished feature of modeling the porous medium as a stationary phase.

In this work, we add to the `upstreamFoam` solver the implementation of an implicit coupled solution for phase fraction equations based on the formulation proposed by Keser et al. [5]. In contrast to the explicit approach, we obtain a better approximation for the phase fractions due to their simultaneous solution, resulting in a more flexible time step size choice, which contributes to the reduction of the computational cost.

The following section presents the mathematical and numerical formulations adopted. Verification tests and an application case are presented in Section 3, followed by Section 4 with final discussions and conclusions.

2 Mathematical and numerical formulations

The primary objective of this work is to develop an application in OpenFOAM that effectively solves multiphase physical systems by the coupling balance equations for phase fractions. The specific focus is on using this solver for porous media flows within the oil and gas industry. The mathematical formulation is based on the Euler-Euler multi-fluid approach, with a particular emphasis on incorporating a specialized treatment for the porous media, treating it as a stationary phase.

In the Euler-Euler formulation, the interaction effects between phases are accounted for in a complete momentum balance equation for each phase, that considers viscous and turbulent stress, interfacial forces, and surface tension [7, 8]. For the purpose of this work, we do not consider such effects and use a simplified version of the referred equation that reduces to the standard Darcy equation:

$$\alpha_i \mathbf{U}_i = -\frac{k_{r,i}}{\mu_i}\mathbf{K} \cdot (\nabla p - \rho_i \mathbf{g}), \tag{1}$$

where the index i represents one phase with fraction α_i, velocity $\mathbf{U}_i$, relative permeability (k_r) in phase i, $k_{r,i}$, viscosity μ_i, and density ρ_i. The tensor $\mathbf{K}$ is the absolute permeability, p is the pressure of the system, and $\mathbf{g}$ is the gravity acceleration. The phase fractions are related to the saturation of classic approaches by

$$S_i = \frac{\alpha_i}{\alpha_v}, \tag{2}$$

being α_v the void fraction or porosity, that satisfies

$$\alpha_v = 1 - \sum_{i=1}^{N_s} \alpha_i, \tag{3}$$

where N_s is the number of stationary phases. Stationary and moving phases are related by

$$\sum_{i=1}^{N} \alpha_i = 1, \tag{4}$$

where $N = N_s + N_m$ denotes the sum of the number of stationary and moving phases.

Considering a system of incompressible phases, the mass balance equation for each phase is:

$$\frac{\partial \alpha_i}{\partial t} + \nabla \cdot (\alpha_i \mathbf{U}_i) = 0, \tag{5}$$

while the mass conservation of the system is:

$$\nabla \cdot (\mathbf{U}_m) = 0, \tag{6}$$

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where $\mathbf{U}_m$ is the mixture velocity which, for N phases, is given by

$$\mathbf{U}_m = \sum_{i=1}^{N} \alpha_i \mathbf{U}_i. \tag{7}$$

The convective term of Eq. (5) can be expanded and expressed in terms of the mixture velocity, resulting in the following expression:

$$\frac{\partial \alpha_i}{\partial t} + \nabla \cdot (\alpha_i \mathbf{U}_m) + \nabla \cdot \left(\alpha_i \sum_{j=1, j\neq i}^{N} \alpha_j (\mathbf{U}_i - \mathbf{U}_j) \right) = 0. \tag{8}$$

In summary, the model for incompressible multiphase flows in porous media consists of a set of partial differential equations given by the Darcy equation, Eq. (1), the total mass conservation, Eq. (6), and the phase fraction equation, Eq. (8).

2.1 Numerical procedure

To solve the non-linear system for pressure, phase velocities, and phase fractions, we use the segregated IMplicit Pressure Explicit Saturation (IMPES) scheme [3], solving pressure and velocity separately from the phase fractions.

Using the total mass conservation, Eq. (6), after summing Darcy's law of each phase, we obtain the pressure equation:

$$\nabla \cdot \left(\sum_{i=1}^{N} \left(\frac{k_{r,i}}{\mu_i} \mathbf{K} \cdot (\nabla p - \rho_i \mathbf{g}) \right) \right) = 0, \tag{9}$$

that is solved by a Pressure IMplicit splitting of operator for Pressure-Linked Equations (PIMPLE) method in OpenFOAM. To approximate the phase fraction equation, Eq. (8), we consider an implicitly coupled procedure presented by Keser et al. [5], and described below.

2.2 Linearization by Keser

The coupled implicit formulation consists of a linear system of equations to describe the relationship between the phase fractions. In this context, some terms of Eq. (8) are non-linear so, it is necessary to linearize them to construct the linear system. To explain the linearization methodology proposed by Keser, we consider the phase continuity equation, Eq. (8), for a three-phase system:

$$\frac{\partial \alpha_i}{\partial t} + \nabla \cdot (\alpha_i \mathbf{U}_m) + \nabla \cdot \left(\alpha_i \sum_{j=1, j\neq i}^{3} \alpha_j (\mathbf{U}_i - \mathbf{U}_j) \right) = 0. \tag{10}$$

When $i = 1$, the non-linear term in the balance equation, Eq. (10), is given by:

$$\alpha_1 \sum_{j=2}^{3} \alpha_j (\mathbf{U}_1 - \mathbf{U}_j) = \alpha_1 \alpha_2 (\mathbf{U}_1 - \mathbf{U}_2) + \alpha_1 \alpha_3 (\mathbf{U}_1 - \mathbf{U}_3), \tag{11}$$

where $\mathbf{U}_1 - \mathbf{U}_2$ is called relative velocity and represented as $\mathbf{U}_{r,1,2}$. Note that the phase velocities do not depend implicitly on the phase fractions, and hence the linearization of the term containing relative velocities around the solution from the previous time-step/iteration reads:

$$\mathbf{U}_{r,1,2} \alpha_1^n \alpha_2^n \approx \mathbf{U}_{r,1,2} \alpha_1^o \alpha_2^o + \left(\frac{\partial (\mathbf{U}_{r,1,2} \alpha_1 \alpha_2)}{\partial \alpha_1} \right)^o (\alpha_1^n - \alpha_1^o) + \left(\frac{\partial (\mathbf{U}_{r,1,2} \alpha_1 \alpha_2)}{\partial \alpha_2} \right)^o (\alpha_2^n - \alpha_2^o) \tag{12}$$

$$\approx \mathbf{U}_{r,1,2} \alpha_1^n \alpha_2^o + \mathbf{U}_{r,1,2} \alpha_1^o \alpha_2^n + \mathbf{U}_{r,1,2} \alpha_1^o \alpha_2^o, \tag{13}$$

where superscripts n and o denote the new and old time step/iteration.

Following this approach, the non-linear term in the phase fraction equation for a general multiphase system can be written as

$$\alpha_i \sum_{j=1,j\neq i}^{N} \alpha_j(\mathbf{U}_i - \mathbf{U}_j) = \underbrace{\alpha_i^n \sum_{j=1,j\neq i}^{N} \alpha_j^o(\mathbf{U}_i - \mathbf{U}_j)}_{\text{implicit}} - \underbrace{\alpha_i^o \sum_{j=1,j\neq i}^{N} \alpha_j^o(\mathbf{U}_i - \mathbf{U}_j)}_{\text{explicit}} + \underbrace{\alpha_i^o \sum_{j=1,j\neq i}^{N} \alpha_j^n(\mathbf{U}_i - \mathbf{U}_j)}_{\text{cross-coupling}}. \tag{14}$$

It is possible to observe that the method proposed by Keser consists of assembling the linear system by dividing the non-linear term into three components: explicit, implicit, and cross-coupling.

3 Numerical Results

In this section, we first test our model in a verification study, then we present an application case. Numerical experiments consider the GAMG (generalized geometric algebraic multigrid) and DIC (diagonal incomplete Cholesky) smoother in a stabilized PCG (preconditioned conjugate gradient) algorithm with a tolerance of 10^{-8} for the pressure system. The system for phase fractions, in turn, uses the OpenFOAM diagonal solver. Concerning the temporal approximation, we use an explicit Euler method with adjustable time step such that

$$\Delta t_{\max} = \frac{C_{max}}{C}, \tag{15}$$

where C is the Courant number restriction, and $C_{\max}$ is user defined.

3.1 Heterogeneous Buckley-Leverett

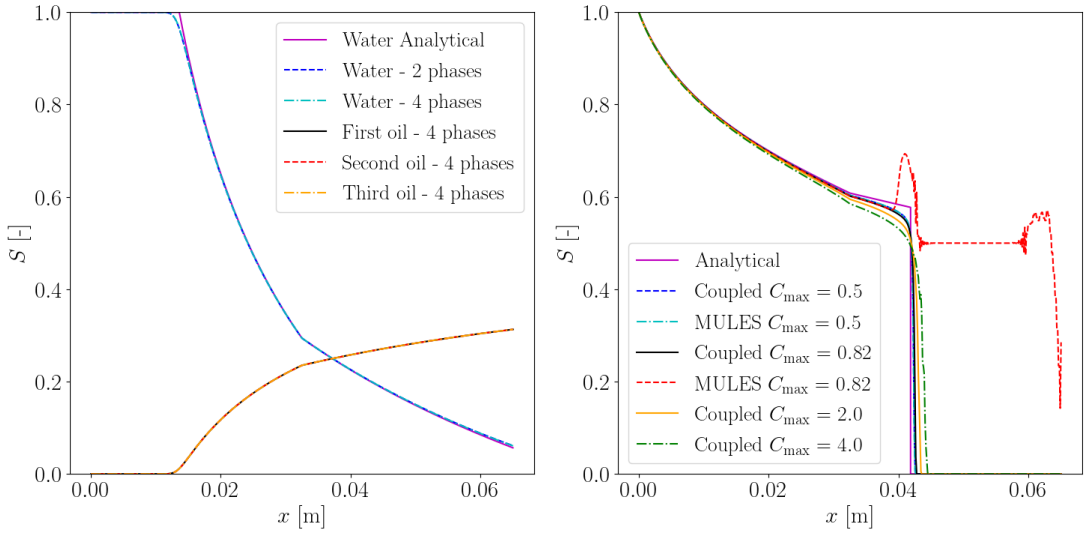
To verify the implemented model, we solve an oil-water flow in a one-dimensional heterogeneous porous medium and compare the results obtained with the Buckley-Leverett semi-analytical solution [11]. We demonstrate the solver capacity to simulate different numbers of moving phases considering two scenarios: one with two moving phases, and the other with four moving phases. Then, we present a test where the coupled implicit solution is compared to an explicit one.

The domain $\Omega = [0, 0.065]$ is considered fully saturated with oil, and water is injected from $x = 0\,\text{m}$ at a constant mass flow rate of $1.67 \times 10^{-5}\,\text{kg/s}$, producing oil and water at $x = 0.065\,\text{m}$, where a fixed pressure of 0.1 MPa is maintained. The void fraction (or porosity) is $\alpha_v = 0.3$ if $0 \leq x \leq 0.0325$ and $\alpha_v = 0.15$ if $0.0325 < x \leq 0.065$, while the absolute permeability is $\mathbf{K} = 101.32\,\text{mD}$. The properties of water (denoted by w) and oil (denoted by o) are: $\rho_w = 1000\,\text{kg/m}^3$, $\mu_w = 0.001\,\text{Pa}\cdot\text{s}$, $\rho_o = 800\,\text{kg/m}^3$, and $\mu_o = 0.002\,\text{Pa}\cdot\text{s}$. In this study, gravity is negligible.

We present in Fig. 1 the saturation profiles after 2000 s considering a computational mesh with 500 cells, for which it has been used the Brooks and Corey relative permeability model with $k_{r,i(\max)} = 1$ for both phases [2]. In the referred experiments, we vary the Brooks and Corey exponent n and the value of $C_{\max}$.

In Fig. 1a, we set $n = 1$ and $C_{\max} = 0.5$ and consider two scenarios: a two-phase flow case, and a four-phase flow case (three separated oil phases with the same fluid properties and equally distributed in the domain). We note that the approximations of both water saturations are close to the analytical solution. Therefore, for the same flow condition, we obtain accurate solutions independently of the number of phases. Additionally, we present the oil saturation curves to confirm that the three oil saturations are equal.

In Fig. 1b, we set $n = 2$ and vary the value of $C_{\max}$ to compare the solution provided by the coupled implicit solver with the explicit approximation for the phase fractions by using the Multi-dimensional Universal Limiter with Explicit Solution (MULES) available in OpenFOAM. Firstly, we observe that the approximations provided by both methodologies are equivalent and accurate for $C_{\max} = 0.5$. For $C_{\max} = 0.82$, the MULES approximation presented instabilities, while the coupled solution proved precise. Instabilities in the MULES solution arise due to its explicit nature, with stability typically limited to $C_{\max} = 0.8$. This behavior has been consistently observed in simulations conducted using the original version of the Euler-Euler application in OpenFOAM. For $C_{\max} = 2.0$, the coupled solution produced a satisfactory result, and presented subtle instabilities for $C_{\max} = 4.0$, when compared to the analytical solution. This study demonstrates a great advantage in terms of the time step size for the coupled model when compared to the MULES solver. Even in a simplified problem, it is possible to increase almost five times the time step.



(a) Two-phase and four-phase flow scenarios. (b) Water saturation by coupled and MULES.

Figure 1: Saturation profiles for the heterogeneous Buckley-Leverett case.

3.2 Application case

In this experiment, we present an application case in a 3D heterogeneous domain to demonstrate the capacity of the solver to handle more complex problems. The domain considered has dimensions of $0.04\,\text{m} \times 0.1\,\text{m} \times 0.04\,\text{m}$ and $40 \times 100 \times 40$ computational cells. It is fully saturated with oil, and water is injected from $y = 0\,\text{m}$ at a constant mass flow rate of $8.32 \times 10^{-5}\,\text{kg/s}$, producing oil and water at $y = 0.04\,\text{m}$, where a fixed pressure of 10 MPa is maintained.

Porosity and absolute permeability fields have been generated randomly, see the illustration in Fig 2. We use the Brooks and Corey relative permeability model with $k_{r,i(\max)} = 1$ and $n = 2$ for both phases, $C_{\max} = 2.0$, the same properties of oil and water considered in the previous study, and gravity is neglected.

We present in Fig. 3 the water saturation at times 200 s, 700 s, and 1200 s, where we observe a behavior compatible with the physics of the flow. We remark that in this configuration fingering instabilities appear at the saturation front and evolve in time, characterizing a complex phenomenon due to the viscosity ratio between the fluids.

Finally, we present in Fig 4 a history of the pressure gradient during the simulation, where it is possible to observe a pressure drop around $t = 1243\,\text{s}$, that corresponds to the breakthrough time (when the water arrives at the outlet). This characterization can be performed by analyzing the time at which the first water flow value occurs at the domain outlet. Note that the breakthrough time estimated is in agreement with the saturation profiles presented in Fig. 3. We remark that the breakthrough time can be important data for decision-making in reservoir engineering.

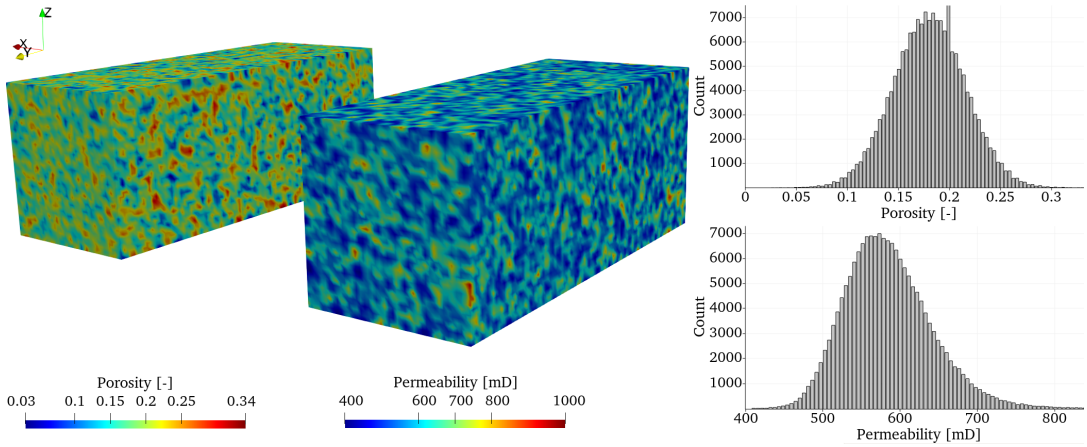


Figure 2: Porosity and absolute permeability for the 3D application case.

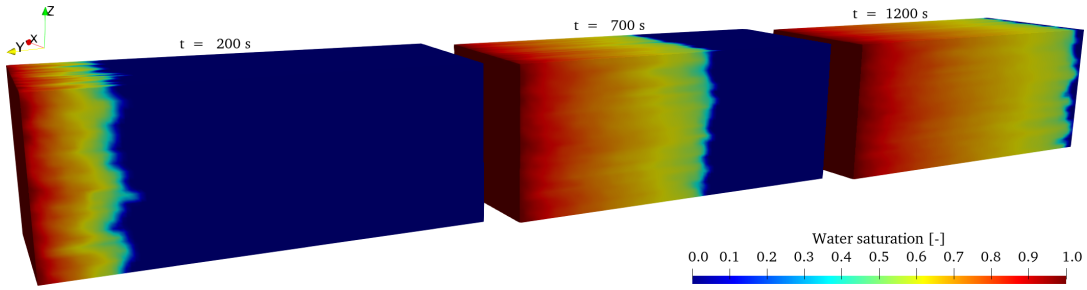


Figure 3: Water saturation profiles of the 3D application case.

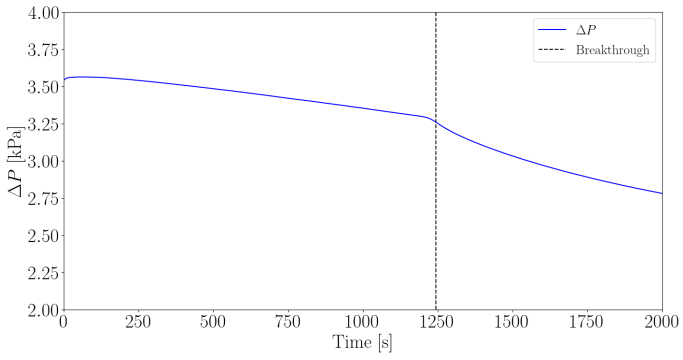


Figure 4: Pressure drop during the simulation.

4 Conclusions

In this work, an OpenFOAM solver with an implicit coupled solution for phase fractions has been developed for multiphase systems where the stationary phases are used to model porous media. Verification tests have been performed in a one-dimensional problem with an analytical solution, obtaining accurate results for the approximation of the saturation front. We showed that the coupled methodology for the solution of phase fractions allows for the use of larger time steps when compared to MULES, being a promising alternative to reduce computational costs. Finally, an application case in a 3D heterogeneous porous medium has been presented, illustrating the ability of the model to simulate more complex problems.

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