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idealCompositionalFoam: An extension to the Darcy-scale compositional solver in OpenFOAM

Content

Compositional modelling of multiphase flow in porous media at Darcy-scale is still in its early development stages in OpenFOAM 1. One critical application of simulating multiphase flow in porous media is in Carbon Capture and Storage (CCS) where the rock and fluids interactions between CO2 and the host environment can be modelled to predict storage performance. The existing gap in OpenFOAM prevents this powerful Computational Fluid Dynamics (CFD) tool from wider applications in decarbonisation and energy transition aspects.

There are a number of porous media flow solvers in OpenFOAM; however, these packages do not account for compositional simulation (multiphase multicomponent flow with phase interactions) in porous media at the large (i.e. Darcy) scale, as relevant in CO2 storage processes. At pore scale, compositional simulation is addressed by GeoChemFoam package 2 which couples OpenFOAM flow transport with PHREEQC species reactive transport. Additionally, a multicomponent formulation is implemented in coupledMatrixFoam [3] at Darcy-scale. However, most Darcy-scale packages follow a Black Oil model that treat phases as separate non-interacting continua, e.g., porousMedia4Foam [4] and porousMultiphaseFoam (PMF) [5]. The most famous module of PMF package is impesFoam that solves for incompressible two-phase fluid flow in porous media using IMPES method. Multiple developments of impesFoam exist, including the compressible solution using upstreamFoam [6], groundwater modeller [7], 3-phase solver [8], adaptive mesh refining model [9], hybrid porous-free flow solver using hybridPorousInterFoam [10] and fractured modeller [11].

In an effort to cover the abovementioned gap, we developed an extension to impesFoam called compositionalIGFoam [1, 12], able to account for CO2/water interactions in CO2 storage processes in aquifers using simplified formulations. In this solver, mass transfer between the phases is handled by Henry's and Raoult's laws by assuming equilibrium at each timestep, and hence, skipping the solution to species transport equations. Here, we further developed compositionalIGFoam by updating this code, where the equilibrium assumption is eased, and the species transport equations are solved at each timestep. In the new extension, called idealCompositionalFoam, a sequential approach is adopted. The process is divided into two stages at each timestep: 1) a fully transport process followed by 2) an equilibration stage where mass transfer between the phases is occurred (water evaporating and CO2 dissolution). In the CO2/water binary system, one transport equation is solved for one component (e.g. CO2) in both gas and liquid phases while the other component is calculated by subtracting that mole fraction from one. During the equilibration, equilibrium values are estimated by flash calculations.

The solver was validated by simulating the injection of CO2 into a water-saturated core model and comparing the results against CMG-GEM. Great agreement was achieved between the two models with only 0.97% and 0.4% difference for water and CO2 mole fraction values in liquid and gas phases, respectively. The choose of more accurate parameters (density / viscosity and Henry's constant values) compared to previous extension resulted in even more accurate results. In summary, the idealCompositionalFoam extension brings more opportunities to OpenFOAM users for modelling compositional multiphase flow in porous media and associated applications.

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Primary author: PAPI, Ali (Research Centre for Carbon Solutions (RCCS))

Co-authors: Dr JAHANBAKHSH, Amir (Research Centre for Carbon Solutions (RCCS)); Dr MARCOS MAGALHÃES, Gabriel (PIEP - Centre for Innovation in Polymer Engineering, University of Minho); Prof. MAROTO-VALER, M. Mercedes (Research Centre for Carbon Solutions (RCCS))

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