



Multiphase Compositional Modelling of CO₂ Injection Under Sub- and Supercritical Conditions

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Modelling of CO₂-H₂O mixture flows in a porous media under subcritical conditions remains a challenging issue for carbon sequestration and possible leakage scenarios. Currently, there is no widely used and generally accepted numerical model that can simulate three-phase flows with both gaseous and liquid CO₂-rich phases. We propose a new compositional modelling approach for sub- and supercritical three-phase flows of water, liquid CO₂ and gaseous CO₂. The new approach is based on the calculation of the thermodynamic potential of the mixture as a function of pressure, total enthalpy and mixture composition and storing it values as a spline table, which is then used for the hydrodynamic simulation. A three-parametric generalisation of the Peng-Robinson equation of state is used to fit the experimental data on CO₂-H₂O mixture properties.

Using the developed approach, we assess several sample problems of CO₂ injection in shallow reservoirs for the purpose of testing the model. We provide the simulation results for a simple 1D problem with a homogeneous reservoir and for a more complicated 2D problem with a highly heterogeneous reservoir using data from the 10th SPE comparative project reservoir. We analyse the temperature variations in the reservoir due to the dissolution of CO₂ in water and the evaporation of liquid CO₂ under subcritical conditions. The interplay of these processes results in a complicated non-monotonic temperature distribution. At different distances from the CO₂ injection point, the temperature can either decrease or increase with respect to the reservoir temperature before injection. The main phenomenon responsible for the considerable temperature decline around the CO₂ injection point is the liquid CO₂ evaporation process.

We also consider parallel simulations of supercritical CO₂ plume evolution at Johansen formation. Firstly, we consider a test scenario using a simplified geological model. Both the free CO₂ phase saturation and the integral parameters of the CO₂ distribution predicted by our approach are in a good agreement with commonly used simulators TOUGH2 and ECLIPSE. Secondly, we consider the plume evolution using a complicated geological model (NPD5 model). For better resolution of the plume, we use local grid refinements. We simulate 100 years of CO₂ injection. The total injection volume is 400 Mt of CO₂. After the injection is stopped, we continue the simulation to evaluate the preferable directions of CO₂ migration in the formation. We analyse the influence of different trapping effects on the storage. Immediately after the well is stopped, the main part of the injected CO₂ is in free mobile phase. Afterward, while CO₂ is migrating upward, the role of residual and solubility trapping is rising. We evaluate an optimized location of the injection well that makes possible a more complete use of anticlines for structural trapping. The optimized location of the well makes possible a more effective trapping of the injected CO₂ in the formation.

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