



Simulation of Multiphase Water-Carbon Dioxide Mixture Flows in Porous Media

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Two-phase models are widely used for simulation of CO₂ storage in saline aquifers. These models support gaseous phase mainly saturated with CO₂ and liquid phase mainly saturated with H₂O (e.g. TOUGH2 code). For deep aquifers where CO₂ injection may result a plume of supercritical CO₂ compositional simulation approach must be applied. This approach originated from petrol reservoir simulation studies is based on a cubic equation of state and is also capable only of single-phase states and two-phase states of liquid-gas type.

The goal of the present study lies in development of a new mathematical approach for compositional simulation of carbon sequestration processes. The approach is supposed to be capable both of single-phase and two-phase states of liquid-gas type as in classical models and also of two-phase states of liquid-liquid type and three-phase states at high pressure. The liquid-liquid states are formed by two liquids. The first liquid is mainly saturated with water while the second is mainly saturated with CO₂. These thermodynamic equilibriums with liquefied CO₂ phase can be detected experimentally (Takenouchi et. al., 1964). The three-phase states represent a composition of the two-phase states of liquid-gas and liquid-liquid types. The three phases are water and CO₂ in liquid and gaseous states. As liquefied CO₂ is negatively buoyant at high pressure the described states can result in non-classical hydrodynamic effects in the aquifer with CO₂ sinking and consequently in non-classical structural trapping scenarios.

The distinctive feature of the proposed approach lies in the methodology for mixture properties determination. Transport equations and Darcy law are solved together with calculation of the entropy maximum that is reached in thermodynamic equilibrium and determines the mixture composition. To define and solve the problem only one function – mixture thermodynamic potential – is required. The proposed approach was implemented in MUFITS (Multiphase Filtration Transport Simulator) code for compositional hydrodynamic simulations. The code was used for 1D, 2D and 3D simulations of carbon dioxide injection in water saturated reservoirs. The sample 1D simulation demonstrates a simple scenario when gaseous CO₂ injection results in underground CO₂ liquefaction and evolution of the three-phase flow zone. The two-phase and three-phase state zones are separated by clearly visible mobile phase discontinuities. The 2D and 3D examples demonstrate different scenarios of CO₂ injection in a folded reservoirs with CO₂ being both only in gaseous state (conventional situation) and in liquid state too. The 10th SPE comparative solution project reservoir was used to test the MUFITS code robustness in simulation of flows in highly heterogeneous reservoir.

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