Multiphase Multicomponent Flow and Reactive Transport (MMF&RT) modeling

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Development of multiphase multicomponent flow (MMF) simulators can be traced all the way back to the 1970s, and that of reactive transport (RT) codes even earlier. Numerous mathematical and numerical methods have been proposed to couple flow and chemical reactions [3]. Efforts have been made to deal with different specific aspects related to the presence of two or more fluid phases and multiple components, such as dis-/appearance, thermodynamic state of mixtures, coupling, and numerical stability. A significant progress has been done in understanding of the physics of the multiphase flow, i.e. estimation of characteristic properties of homogeneous and heterogeneous porous media. Due to the physical and numerical complexity of the MMF&RT, the problem is often simplified supposing non-reactive components, phases, or loose coupling. Until recently, the gas phase was systematically presented by one gas species only. In models of impure CO_2 injection [1], the gas phase consisted by CO_2(g) . The co-injected impurities were supposed dissolved in brine, hence, the additional amount of brine was injected that changes chemical reactions, fluxes and mass balance. Accurate modeling of phases, of their thermodynamic properties and fluxes is required to describe real aqueous and gas mixtures. Such calculations are numerically demanding because of high degree of freedom. We demonstrate the operator-splitting based approach used in the reactive transport simulator HYTEC for the compressible EOS-based MMF&RT [2]. Modeling of experimental, numerical, and field cases of injection of CO_2 with impurities or tracers show highly coupled physical processes related to complex phase composition, e.g. density driven flow and chromatographic partitioning,

References

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