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PROBABILITY DENSITY FUNCTION (PDF) APPROACH FOR MODELING NON-EQUILIBRIUM GRAVITY-DRIVEN FLOWS IN POROUS MEDIA

Manav Tyagi[†] and Patrick Jenny

Institute of Fluid Dynamics, ETH Zurich
Sonneggstrasse 3, Zurich 8092, Switzerland

[†]e-mail: tyagi@ifd.mavt.ethz.ch, web page: http://www.ifd.mavt.ethz.ch

Summary. Many of the complex physical processes relevant for compositional multi-phase flow in porous media are well understood at the pore-scale level. In order to study CO_2 storage in sub-surface formations, however, it is not feasible to perform simulations at these small scales directly and effective models for multi-phase flow description at Darcy scale are needed. Unfortunately, in many cases it is not clear how the micro-scale knowledge can rigorously be translated into consistent macroscopic equations. Recently, we proposed a new probability density function (PDF) based methodology, which provides a link between Lagrangian statistics of phase particle evolution and Darcy scale dynamics (Tyagi et al. *JCP* 2008). Unlike in a deterministic method, the evolution of Lagrangian stochastic particles representing small fluid phase volumes is modeled. Each particle has a state vector consisting of its position, velocity, fluid phase information and possibly other properties like phase composition. While the particles are transported through the computational domain according to their individual velocities, the properties are modeled via stochastic processes honoring specified Lagrangian statistics.

Here we employ the PDF-approach for modeling multi-phase flow with interfacial mass transfer (dissolution) in a porous medium. The statistics of flow is respresented by a joint probability density function (JPDF), which evolves in a high dimensional space via Fokker-Planck equation. The drift and diffusion coefficients in the Fokker-Planck equations are the conditional stochastic moments of stochastic processes. To demonstrate the concept, we consider an example of two-phase immiscible CO_2-brine flow with non-equilibrium dissolution of CO_2 into brine. The brine with dissolved CO_2 is denser than pure brine and sinks down, which leads to dissolution-driven gravity currents. The Fokker-Planck equation is solved with our recently developed stochastic particle method for multi-phase flow (Tyagi et al. *JCP* 2008). We also derive transport equations for the stochastic moments (mean, variance, etc.) and show that unlike the Fokker-Planck equation the resulting system of moment equations is unclosed. In the traditional Darcy formulation, for example, the transport equation for the average concentration is closed by neglecting the variance. However, with several one- and two- dimensional simulations it is shown that the PDF and Dacry modeling

approaches give significantly different results. While the PDF-approach properly accounts for the long correlation length scales and the concentration variance in dissolution driven gravity currents, this phenomenon cannot be captured accurately with a standard Darcy model.