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Modeling non-Fickian dispersion by use of the velocity PDF on the pore scale

Sheema Kooshapur and Michael Manhart
Fachgebiet Hydromechanik, Technische Universitaet Muenchen, Meunchen, Germany

For obtaining a description of reactive flows in porous media, apart from the geometrical complications of resolving the velocities and scalar values, one has to deal with the additional reactive term in the transport equation. An accurate description of the interface of the reacting fluids – which is strongly influenced by dispersion- is essential for resolving this term. In REV-based simulations the reactive term needs to be modeled taking sub-REV fluctuations and possibly non-Fickian dispersion into account.

Non-Fickian dispersion has been observed in strongly heterogeneous domains and in early phases of transport. A fully resolved solution of the Navier-Stokes and transport equations which yields a detailed description of the flow properties, dispersion, interfaces of fluids, etc. however, is not practical for domains containing more than a few thousand grains, due to the huge computational effort required. Through Probability Density Function (PDF) based methods, the velocity distribution in the pore space can facilitate the understanding and modelling of non-Fickian dispersion [1,2].

Our aim is to model the transition between non-Fickian and Fickian dispersion in a random sphere pack within the framework of a PDF based transport model proposed by Meyer and Tchelepi [1,3]. They proposed a stochastic transport model where velocity components of tracer particles are represented by a continuous Markovian stochastic process. In addition to [3], we consider the effects of pore scale diffusion and formulate a different stochastic equation for the increments in velocity space from first principles.

To assess the terms in this equation, we performed Direct Numerical Simulations (DNS) for solving the Navier-Stokes equation on a random sphere pack. We extracted the PDFs and statistical moments (up to the 4th moment) of the stream-wise velocity, u, and first and second order velocity derivatives both independent and conditioned on velocity. By using this data and combining the Taylor expansion of velocity increments, du, and the Langevin equation for point particles we obtained the components of velocity fluxes which point to a drift and diffusion behavior in the velocity space. Thus a partial differential equation for the velocity PDF has been formulated that constitutes an advection-diffusion equation in velocity space (a Fokker-Planck equation) in which the drift and diffusion coefficients are obtained using the velocity conditioned statistics of the derivatives of the pore scale velocity field. This has been solved by both a Random Walk (RW) model and a Finite Volume method. We conclude that both, these methods are able to simulate the velocity PDF obtained by DNS.

References
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