Contribution ID: **461** Type: **Oral Presentation**

A Lagrangian Simulation Framework for Multiphase Flow and Transport in Fractured Porous Media

Wednesday, 15 May 2024 11:25 (15 minutes)

Particle tracking schemes, including random walk (RW)-based methods, are attractive for modeling advective transport, since they do not suffer from numerical diffusion [Salamon et al. (2006)][1]. In scenarios involving multi-species transport, these schemes meticulously capture the degree of spatial mixing across all scales. With such schemes, one can leverage thermodynamic rate laws which when applied to particles in close proximity result in realistic reaction rates. This stands in contrast to classical upscaling-based approaches which assume complete mixing and may not accurately model small-scale variations in reaction rates [Ding et al. (2013)][2].

We present an improved stochastic particle method in the context of multiphase transport in fractured porous media. Our study focuses on limit case scenarios where the microscopic processes, such as capillary diffusion and pore-scale dispersion, do not exert significant influence at the macroscopic levels. For a time-varying system that exhibits a potential solution discontinuity, such as the aforementioned one developing saturation jumps, Lagrangian models may face challenges in producing physically meaningful solutions. Here, we choose a regularization approach based on artificial diffusion/dissipation, and incorporate an adaptive diffusion coefficient. This coefficient is active only in the vicinity of saturation fronts, as is dictated by its saturation-gradient-dependent scaling, which has been conceptualized in Monga et al. (2022)[3]. Moreover, guided by the vanishing viscosity solution of the 1-D Buckley-Leverett problem, the diffusion coefficient was found to scale with the characteristic speeds of the original hyperbolic system.

We demonstrate that the particle tracking scheme accurately captures sharp saturation profiles in a 1-D Buckley-Leverett reference problem. Subsequently, we analyse the particle-based results in the context of a realistic 2-D fracture network embedded in a permeable matrix. In order to extend the applicability of the proposed regularization approach, isotropic and anisotropic variants of the diffusion coefficient tensor, respectively, are assessed for flow scenarios involving, e.g., gravitational effects and heterogeneity in the matrix. Further application areas include the modeling of physical sub-grid effects, such as dissolution of one phase into the other [Tyagi (2011)][4] and precipitation-dissolution type reactions.

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Session Classification: MS07

Track Classification: (MS07) Mathematical and numerical methods for multi-scale multi-physics, nonlinear coupled processes