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Dissipative Particle Dynamics Based Mesoscale Modeling of Multiphase Flow in Reconstructed High-Resolution Nanoporous Shale Pore Networks

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Numerical modeling has been an increasingly important approach for better understanding fluid flow and transport phenomena in organic-rich, nanoporous shale. However, deployment of numerical models in the context of nanoporous shale is challenging because of the multi-length-scale nature of the porosity in shale, where pore sizes can range between the nanoscale (~ 10^{-9} m) and microscale (~ 10^{-6} m), because of the complex physical and chemical interaction between fluid and wall surfaces in pores, and because of the demanding computing costs required for simulations to reach the desired spatial and temporal scales. For example, simulations of pore-network fluid flow in a representative region of interest (ROI) in a micro core sample are beyond the current computational limit of the molecular dynamics models, and also immature with the particle-differential-equations based continuum computational fluid dynamics models. The class of dissipative particle dynamics (DPD) models, which were originally introduced for the modeling of microscopic hydrodynamics, have recently been extended and applied for mesoscale flow and transport in porous media. A remarkable feature of the DPD models is that they are able to reproduce some of the key characteristics of fluids at both the molecular and continuum scales, which make these models more flexible for modeling multi-length-scale fluid systems. Among the many variances of DPD models, the many-body DPD (mDPD) model has demonstrated particular suitability for modeling pore-network flow and transport. In the authors' earlier work [Xia et al., 2017, *Physics of Fluids* 29(5)], a modeling & analysis workflow that integrates the digital rock physics to a parallel mDPD code was developed for simulating multiphase flow in shale, where a focused ion beam scanning electron microscope (FIB-SEM) digital imaging process is used to provide voxel data to inform the construction of wall surfaces of the connected pores in the simulations. In the present work, an improved mDPD model for the workflow will be presented, in which an enhanced non-/partial-slip boundary condition algorithm [Li et al., 2017, *Journal of Computational Physics*] will be applied for better resolving wall-fluid interactions in the multiscale pore networks of shale. Moreover, in order to reduce load imbalance in parallel computing with massive CPU nodes and hence realize the mDPD flow simulations in shale ROIs at a desirably larger spatial and temporal scale, a node-level multithreading parallelism will be implemented in our MPI parallel mDPD code, and deployed along with a recursive coordinate bisection (RCB) based adaptive domain repartitioning algorithm. Simple flow simulations in manufactured slit nanopores will be presented for verification and validation of the improved workflow. Multiphase flow simulations that contain hundreds of millions of mDPD particles will then be presented for permeability-fluid dependence study in the reconstructed high-resolution nanopore networks of a selected shale ROI. Simulation results and computational performance will be reported and analyzed. The workflow developed in the present study is still relatively new in the area of virtual rock analysis, especially for nanoporous shale. Nevertheless, it is being continuously improved toward a robust and accurate mesoscale model that is expected to bridge the gap between its molecular- and grain-scale counterparts.

References

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