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# A Rigorous Upscaling Procedure to Predict Macro-scale Transport Properties of Natural Gas in Shales by Coupling Molecular Dynamics Simulation with Lattice Boltzmann Method

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It is well know that shale formations exhibit multi-scale geological features such as nanopores in the formation matrix and natural fractures at multiple length scales. The key challenge in unconventional reservoir simulations thus is how to preserve fine-scale information in coarse-scale reservoir simulations for correct production forecasting and reserve estimation. In this paper, we present an upscaling procedure by coupling Molecular Dynamics (MD) simulation and lattice Boltzmann method (LBM) with digital rock reconstruction techniques to predict transport properties of natural gas in shales at different length scales. The proposed approach allows calculating macro-scale transport properties of natural gas in shales for unconventional reservoir simulations without losing critical fine-scale (nano-scale) information.

The reconstructions of multi-scale shale samples are performed using digital rock imaging techniques, i.e. FIB-SEM, Nano-CT and Micro-CT. These experiments provide micro-scale pore architectures (~nm), meso-scale mineralogical distribution (~μm), and macro-scale natural-fracture network (~cm), respectively. These multi-scale observations are then utilized for multi-scale digital rock reconstructions for the investigations of multi-scale transport properties. The present upscaling process can be summarized as three steps. First, micro-scale transport properties in organic and inorganic digital rocks from FIB-SEM are calculated using the non-equilibrium MD simulations. Representative organic (kerogen) and inorganic (montmorillonite, kaolinite, etc.) molecules are built upon their molecular structures. Transport properties determined from MD simulation are then served as input parameters for LBM simulations. Second, micro-scale properties of each component are mapped stochastically on its corresponding voxels in Nano-CT digital rocks. The meso-scale permeabilities of Nano-CT digital rocks are then calculated using the generalized LBM model. Last, the effective permeabilities of the macro-scale shale samples (Micro-CT) with micro-fracture networks are calculated using the generalized LBM model, in which the matrix permeabilities are obtained from the step 2.

In the simulation results, the effective permeability changes significantly (up to 10 times) for different shale samples. The difference in permeability is attributable mainly to porosity, organic content and fracture characteristics. It is found that the effective permeability increases when the organic content is increased, and better pore connectivity in organic matters also enhances the effective permeability.

**Keywords**: shale gas, molecular simulation, lattice Boltzman Method, digital rock