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An integrated fractional partial differential equation and molecular dynamics model of anomalously diffusive transport in heterogeneous nano-pore structures

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ABSTRACT

Fluid flows confined in nano-pore structures exhibit physical behaviors that are not observed in large-scale structures. Molecular dynamics simulation has been used for modeling nano-scale fluid flows at nanoscale, but is deemed to be computationally very expensive and is often limited to problems with simple geometry.

We develop an integrated fractional partial differential equation and molecular dynamics upscaling modeling of anomalously diffusive transport in heterogeneous nano-pore structures, which has a significantly improved computational efficiency and memory requirement over the molecular dynamics simulation. Representative applications demonstrate the usage of the new model, which takes the model a few hours on a laptop that would otherwise require a molecular dynamics simulation in the matter of at least 100 years of CPU time on a parallel computer.

1. Introduction

Shale gas has recently become an increasingly important energy resource in the world. However, the underlying mechanism in shale gas recovery is far from being well understood and requires thorough analysis. The fundamental reason is that shale formation often has insufficient permeability due to the existence of nano-pores, which results in a large amount of adsorbed gas and significant decrease of flow rate to the wellbore. Consequently, fluid flows in confined nano-scale structures tend to exhibit physical behaviors that are not observed in large-scale structures. At this scale, the molecular mean free path is comparable to the characteristic pore size, resulting in a large Knudsen number [43]. A recent observation reveals that the flow rate can differ significantly from those predicted by conventional hydrodynamic theory in nanotube membrane [26,34].

The fundamental objective in mathematical modeling of shale gas production is to understand the complex fluid flow processes in confined nano-scale shale formation sufficiently well to optimize shale gas recovery. To do so, one must be able to predict the performance of the reservoir under various exploitation schemes such as hydraulic fracturing and multi-stage horizontal drilling. This is extremely challenging due to the presence of multi-scale porous features and compositional heterogeneity of the subsurface rocks (e.g. organic matters, inorganic clays, etc). Hence, thorough understanding of nano flow is of crucial importance and is urgent because of a significantly increasing need of shale gas production [6,10,11,24,28].

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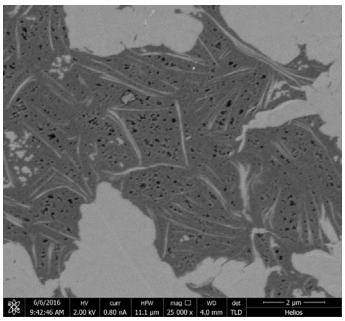

Fig. 1. SEM image of shale rock samples. The dark gray represents the organic matters in shale and the black represents the nano-pores within the organic matters.

In this paper we develop an integrated fractional partial differential equation (FPDE) and molecular dynamics (MD) upscale modeling of anomalous diffusive transport in heterogeneous nano-pore structures. The investigation of gas transport mechanisms in nano-confined spaces facilitates large-scale rock and fluid property characterizations and provides fundamental insights for understanding experimental results from core analysis. The rest of the paper is organized as follows. In section 2 we discuss the application of MD simulation in the anomalously diffusive transport of shale gas molecules in heterogeneous nano-pore structures. In section 3 we present an FPDE to model the anomalously diffusive transport of shale gas and discuss its efficient numerical solution. In section 4 we develop an integrated FPDE-MD upscaling modeling of anomalously diffusive transport of shale gas molecules in digital rock with heterogeneously distributed nano-scale pores. In section 5 we study representative model applications and conduct sensitivity analysis.

2. An MD simulation

It has been found via the use of pore size distribution measurement and high-resolution (up to 3 nm) imaging-technology that the size of the nanopores in shale formation can vary in a wide range and the distribution of the nanopores is highly disordered [31,32,56] (and Fig. 1). These pores can be further categorized into micropores (<2 nm), mesopores ($2 \sim 50$ nm) and macropores (>50 nm) [3,19,45]. Their transport properties depend heavily on the degree of heterogeneity of the pore structures, such as the fraction of different-sized pores and the connectivity between the pores. Within such hierarchical pore structures, advection–diffusion process dominates gas transport behavior in mesopores. As the pore size decreases to microscale, diffusion starts to dominate gas transport [25]. To date, there are few rigorous tools to quantitatively correlate gas transport properties with the morphology of porous media. The investigation of gas transport mechanisms in nano-confined spaces with various pore structures is vitally essential. It facilitates large-scale rock and fluid property characterizations and provides fundamental insights for understanding experimental results from core analysis.

MD tracks the position and velocity of each molecule following Newton's second law of motion [18]. The interaction parameters between different molecules, i.e. the intermolecular potentials, are determined and parameterized from experiments [9,35,36,53]. MD simulation has proven to be a rigorous approach for modeling fluid flow in nano-pore structures [4,8,39,46,54,55]. However, application of MD simulation requires numerical computations of a system that is at the size comparable to the real experimental samples and contains hierarchical pore structures. This can be computationally very expensive, which may restrict the application of MD simulation. Therefore, the development of an alternative, computationally manageable modeling technique is of crucial importance in obtaining effective upscaled transport property of shale formation.

In MD simulation nano-confined space is typically modeled based upon simple pore geometries (e.g. parallel plates or tube) [2,14,34,47] and microporous media (e.g. microporous silica [33], disordered carbon [46], zeolite [48,51]). Periodic boundary conditions are commonly applied. Consequently, MD simulation often has limited capability in capturing the impact of hierarchical pore structure on fluid transport properties [22].

For a heterogeneous porous medium with moderate confinement, fluid particles can easily move through the pores and behave as a normal diffusion [19]. When the confined effects increase, the interaction between rock and gas molecules dominates the transport process. A large quantity of gas molecules may get absorbed to the micropores in rock [46,52]. Thus, the travel time of the adsorbed gas molecules may deviate from that of the gas molecules in the bulk phase [58], leading to a subdiffusive transport that is characterized by a sublinear growth of the particle's mean square displacement $< r^2 >$ with respect to the time t [5,7,39,44]. The limiting case occurs when the size of the pore is comparable to that of particles, which exhibits single-file diffusion that has a time dependence of the mean square displacement to an order of $1/2$, i.e., ($< r^2 > \sim t^{1/2}$) [20,21]. As the confinement gets relaxed, the time dependence of the mean square displacement goes to the order between $1/2$ and 1 [1].