## Integrated multiscale modeling of fluid flow in shale: molecular-to-core scales

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## Abstract

One of the great challenges in modeling fluid flow in shale system is the existence of heterogeneities at different scales. Heterogeneity is not new to researchers studying reservoir characterization. However, in shale strata heterogeneities exist at different scales, i.e., from molecular scale to multiwell scale. While the goal is to predict gas and oil production in a section of reservoir (single well or multiple wells), we learned that processes at very small scale control the production at well scale. We have started a comprehensive research to integrate porosity and permeability, hence fluid flow at different scales. The research includes numerous mathematical and numerical models along bench experiments to validate our models (Figure 1).

*Molecular scale.* At the molecular scale we study the interaction of fluid molecules (gas and liquid, hydrocarbons and aqueous) with pore inner walls [1]. The molecular scale research provides slip coefficients for further implementation in fluid flow models. We also perform extensive molecular dynamics simulations (MD) to study fluid molecules interactions with pore walls. MD reveals many interesting features of fluid flow at confined condition, i.e., very small pores [2]-[4].

*Pore scale.* At the pore scale, the research includes extensive SEM image analysis of the organic matter patches and pores in organic and inorganic. SEM images reveal the locale of the pores and by using image analysis we extract important information about pore geometries in shale system that can be used in fluid flow models [5]-[7].

*Powder scale.* In addition to the direct observation of pores via SEM imaging, we utilize high pressure mercury injection capillary pressure (MICP) and low pressure nitrogen sorption tests to learn about porosity and pore size distribution in shale samples. We also measure permeability of the powder samples by GRI permeability method.

*Core scale.* At the core scale, we measure permeability of the samples using pulse decay permeability and Boyle's law porosity measurements [8].

*Molecule-to-core.* In order to link all these measurements at different scales, we developed different fluid flow models. Information about pore size distribution, pore geometry, porosity, and TOC are input data in our models and apparent permeability is the model prediction. Permeability is the most important and probably most complicated characteristic of shale system. Shale samples show heterogeneity at different scales, e.g., patches of organic matter in the shale system show different pores sizes and wettability. We present a realistic model that honors heterogeneity of organic matter patchiness and its effect on apparent permeability. We use a stochastic classification method based on a

mixture of Gaussian assumption to separate two distributions of pores in organic matter and inorganic matrix. We construct an ensemble-based stochastic model conditioned to total organic content (TOC) and the characteristics of pore-size distributions in both organic and inorganic media [9]. We incorporate a novel permeability model [8] for shale rock that overcomes the limitation of Maxwell slip condition and includes higher order slip effects on gas flow. We validated our model using a set of detailed experimental data on shale samples. These results suggest that heterogeneity at small scale could affect the permeability at core scale and pore sizes corresponding to each compartment; organic and inorganic should be considered to estimate permeability. The model results also confirm permeability enhancement during sorption process in organic matter below critical sorption pressure.

**Keywords:** Langmuir sorption isotherm, gas flow, Knudsen diffusion, slip flow, nanopore, pore size distribution

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Figure 1. Integrated multiscale study of fluid flow in shale system; from molecular scale to core scale.