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Apparent permeability prediction of organic shale with generalized lattice Boltzmann model considering surface diffusion effect

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ABSTRACT

Gas flow in shale is associated with both organic matter (OM) and inorganic matter (IOM) which contain nano-pores ranging in size from a few to hundreds of nano-meters. In addition to the non-continuum effect which leads to an apparent permeability of gas higher than the intrinsic permeability, the surface diffusion of adsorbed gas in organic pores also can influence the apparent permeability through its own transport mechanism. In this study, a generalized lattice Boltzmann model (GLBM) is employed for gas flow through the reconstructed shale matrix consisting of OM and IOM. The Expectation–Maximization (EM) algorithm is used to assign the pore size distribution to each component, and the dusty gas model (DGM) and generalized Maxwell–Stefan model (GMS) are adopted to calculate the apparent permeability accounting for multiple transport mechanisms including viscous flow, Knudsen diffusion and surface diffusion. Effects of pore radius and pressure on permeability of both IOM and OM as well as effects of Langmuir parameters on OM are investigated. The effect of total organic content and distribution on the apparent permeability of the reconstructed shale matrix at different surface diffusivity is also studied. It is found that the influence of pore size and pressure on the apparent permeability of organic matter is affected by the surface diffusion of adsorbed gas. Moreover, surface diffusion plays a significant role in determining apparent permeability and the velocity distribution of shale matrix.

1. Introduction

Shale gas reservoirs contain a significant proportion of hydrocarbon energy, and the successful exploitation of such resource plays an increasingly important role in meeting world's demand for natural gas. Organic shale is known to be fine grained sedimentary rocks consisting of inorganic matter (IOM) and organic matter (OM) with pore sizes ranging from nano- to meso- scale [1,2], in each component of which are involved different flow mechanisms [3]. In the literature, gas flow on nano- to micro-scale in shale is often referred to as rarefied gas flow [4], where the mean free path of gas is comparable to the characteristic length of the micro-pores or throats. Gas flow in shale matrix usually leads to a deviation from the continuum theory [5]. Moreover, previous studies have confirmed that the amount of adsorbed gas constitutes about 20–80% of the total gas in place of shale gas reservoir [6–8], and the surface diffusion of adsorbed gas is an important transport mechanism in these reservoirs [9,10]. A physics-based understanding of gas transport mechanism in shale including non-continuum behaviors and surface diffusion is essential for the development of accurate descriptive transport simulators to predict fluid flow and transport in shale.

For decades, the problem of modeling gas transport in narrow pores and confined spaces in shale has attracted considerable attention among petroleum engineers. Generally speaking, two approaches have been proposed to describe the gas transport and to calculate apparent permeability of organic shale. The first approach is to modify the non-slip boundaries in continuum model by accounting for slip boundary conditions. Beskok and Karniadaki [11] derived a unified Hagen–Poiseuille-type formula to take account of slip flow, transition flow and free molecular flow. Later, Civan [12] and Florence et al. [13] proposed different forms of rarefaction coefficient in Beskok–Karniadaki model. Xiong et al. [14] introduced a capillary model by adding the mass transfer of adsorbed gas into Beskok–Karniadaki empirical equation to study the impact of the adsorbed gas and surface diffusion on gas apparent permeability. The second approach is the superposition of various transport mechanisms. Javadpour [3] combined slip flow and Knudsen diffusion into gas flux equation and derived an

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equation for apparent permeability. Freeman et al. [15] applied dusty gas model (DGM) to account for Knudsen diffusion in shale gas reservoir. Singh et al. [4] combined viscous flow with Knudsen diffusion in their non-empirical apparent permeability model (NAP), and validated the model with previous experimental data. The results show that the NAP can be used for Kn less than unity. Wu et al. [9] further proposed two weighted factors for viscous flow and Knudsen diffusion, respectively. The surface diffusion was also considered in their apparent permeability model.

The limitation of the application of analytical or semi-analytical models to gas flow in porous media is that the pore structure is usually relatively simple, such as capillaries [3,4,14]. Such simplification might produce erroneous results because the pore structures in shale are very complex, as detected by well-established characterization techniques such as SEM [1,16]. To improve this, different pore-scale models have been proposed to link the micro-structure of the porous media with fluid flow characteristics. Among them, the lattice Boltzmann (LB) method has gone through significant improvements over the past years and has become a viable and efficient substitute for conventional N–S solvers in many flow problems especially porous flow and multiphase flow [17]. Because of its inherent kinetic nature, the LB method has attracted huge interest in its extension to simulating micro-gaseous flows, and tremendous efforts have been made to advance the LBM since 2002 [18–20]. With the implementation of appropriate slip boundary conditions and/or effective relaxation time, the LBM was successfully extended for simulation of gaseous flows in slip flow and transition flow regimes, and these LBM approaches have been applied to study gas transport in shale gas reservoir [21–23]. However, because of the complexity of boundary conditions, most of the applications of the slip-based LBM are limited to single channel or bundle of channels [23]. Recently, Chen et al. [20,24] proposed a LB model based on the Dusty gas model (DGM) to predict the apparent permeability of shales with complex porous structures, where the complexity of the slip boundary conditions are avoided. Very recently, Chen et al. [25] improved the generalized lattice Boltzmann model (GLBM) proposed by Guo and Zhao [26] for fluid flow through porous media by including the Klinkenberg effect, and performed several simulations based on heterogeneous shale matrix with natural fractures, organic matter and inorganic minerals [25,27].

In this study, we present a novel adaptation of the GLBM with slip effect proposed by Guo and Zhao [26] and Chen et al. [25] for micro-gas flow in 2-dimensional (2-D) porous shale with surface diffusion further considered. The novelty of the present study is the use of the DGM-generalized Maxwell–Stefan (GMS) approach to calculate the local permeability taking the adsorbed gas and surface diffusion into account. The rest of the paper is as follows. The mathematical and numerical models for predicting apparent permeability of organic shale is introduced in Section 2, and the validation of numerical models is also shown in this section. In Section 3, firstly the permeability of IOM and OM are discussed, and then the effects of component distribution and organic content on apparent permeability of reconstructed shale sample are analyzed. Finally, some conclusions are drawn in Section 4.

2. Model description

2.1. Dusty gas model and generalized Maxwell–Stefan model

The transport of non-adsorbable gas through porous media is in general caused by concentration or pressure gradients. It has been confirmed experimentally and mathematically that the corresponding fluxes can be calculated with high accuracy using the DGM or Knudsen-like theory [28]. However, most recent studies indicate that the above applications have failed to model the gas transport in the presence of the adsorbed gas [29]. To take account of the adsorbed gas effect, Krishna and co-workers [30,31] extended the Maxwell–Stefan formulation in the spirit of the DGM by introducing a generalized Maxwell–Stefan model (GMS) for surface diffusion of adsorbed gas (see Fig. 1). With the premise that the DGM appropriately describes the transport in the "quasi-bulk" phase located in the pore space whereas the GMS describes gas molecular transport at the surface, the total molar flux is expressed by:

$$N_{total} = N_{DGM} + N_{GMS}, \tag{1}$$

where N_{DGM} is the contribution to the flux from the DGM (mol m^{-2} s^{-1}), in which adsorption and surface diffusion is ignored, and N_{GMS} is the contribution from the GMS for surface diffusion (mol m^{-2} s^{-1}). Detailed descriptions of DGM and GMS are given in the next two subsections, respectively.

2.1.1. Dusty gas model

The DGM is based on the combination of the Maxwell–Stefan diffusion equations and the characteristics of mass transfer in porous media. The basic idea of DGM is to consider the solid as a dummy species of infinite mass, which is constrained by unspecified external forces and has zero drift velocity. For a single species i in a n-component mixture the following flux equation of the DGM holds [32]:

$$-\frac{P}{RT}\nabla x_i - \frac{x_i}{RT}\left(1+\frac{K_0}{\eta D_{K,i}}P\right)\nabla P = \sum_{j=1,j\neq i}^{n}\frac{x_j N_i - x_i N_j}{\varepsilon/\tau D_{ij}^0} + \frac{N_i}{D_{K,i}}, \tag{2}$$

where P is pressure (Pa), R is the universal gas constant (8.314 J K^{-1} mol^{-1}), T is temperature (K), η is dynamic viscosity (kg m^{-1} s^{-1}), x_i is the molar fraction of species i, D_{ij}^0 is the binary molecular diffusivity in gas phase (m^2/s), and ε/τ is the ratio of porosity to tortuosity. The Knudsen diffusivity $D_{k,i}$ of species i is defined as:

$$D_{K,i} = \frac{4}{3}K_c\sqrt{\frac{8RT}{\pi M_i}}, \tag{3}$$

where M_i is the Molecular weight of species i (kg/mol). In the case where the pore space is assumed to have a diameter d_p (m), the values of Knudsen coefficient, K_c and the permeability of the porous medium quantifying the viscous flux, K_0 can be related as [33]:

$$K_c = \frac{8}{d_p}K_0 = \frac{\varepsilon}{\tau}\frac{d_p}{4}. \tag{4}$$

If the system contains only one species, Eq. (2) can be simplified as:

$$N_{DGM} = -\frac{1}{RT}\left(D_K + \frac{K_0}{\eta}P\right)\frac{\partial P}{\partial r}. \tag{5}$$

2.1.2. Generalized Maxwell–Stefan model

The GMS model is based on the assumption that the movement of species is caused by a driving force balanced by the friction that the moving species experience both from each other and from their surroundings. The diffusion of adsorbed species satisfies [31]:

$$-\frac{\theta_i(1-\varepsilon)}{RT}\nabla\mu_i = \sum_{j=1,j\neq i}^{n}\frac{\theta_j N_i^s - \theta_i N_j^s}{\rho_p q_{sat} D_{ij}^s} + \frac{N_i^s}{\rho_p q_{sat} D_i^s}, \tag{6}$$

where μ_i is the chemical potential of i (J/mol), θ_i is the fractional coverage, ρ_p is the density of particle or solid skeleton (kg/m^3), q_{sat} is the saturation surface concentration (mol/m^3), D_{ij}^s is the Max-