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Full Length Article

A diffusion–viscous flow model for simulating shale gas transport in nano-pores

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HIGHLIGHTS

- A new model for gas transport in nano-pores is developed.
- The model is based on the Extended Navier–Stokes Equations.
- The mass flux contributed by different flow mechanisms is analyzed by varying K_n.
- The effect of the ratio coefficient, pore size and pressure is investigated.
- The model is validated with DSMC data and by experimental data.

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ABSTRACT

A model for gas flow in nano-pores was developed based on the extended Navier–Stokes equations with the assumption of neglecting adsorption and desorption. The model describes multiple flow regimes, including continuum regime, slip flow regime, transition regime, as well as molecular regime. The total mass flux includes a convective motion term and a diffusion mass transport term. The latter was obtained as a weighted superposition of bulk and Knudsen diffusion. The mass flux, contributed by different transport mechanisms, was analyzed by varying the Knudsen number (ratio between mean free path of the molecules and the pore diameter). The effect of the ratio coefficient (the power-law exponent in the relation between bulk and Knudsen diffusion), the pore size and the pressure on the gas transport was investigated using the proposed model. The predictions of the newly developed model are in good agreement with the Direct Simulation Monte Carlo (*DSMC*) method and with the results of the experiments. Our results show that: (1) As the Knudsen number increases, the contribution of viscous flow to gas transport decreases monotonically, bulk diffusion increases to a peak, and then decreases, whereas the Knudsen diffusion increases monotonically. (2) For a larger ratio coefficient, the bulk diffusion changes more rapidly and the peak is higher. The changing trend of the bulk diffusion is opposite to the Knudsen diffusion. (3) The pressure range in which the viscous flow dominates becomes larger and the peak of bulk diffusion is smaller in larger pores. When the pore pressure is higher, the viscous flow and the bulk diffusion tend to dominate.

1. Introduction

Gas flow in nano-pores plays an important role in many applications including catalysis, molecular sieving and extraction of natural gas from shales. Nano-pores with diameters ranging from a few nanometers to several hundred nanometers are abundant in shale gas reservoirs [1]. This causes a significant difference from conventional gas reservoirs in terms of pore scale and transport mechanisms [2]. In conventional reservoirs continuous flow is dominant, whereas in shale gas reservoirs gas can flow in nano-pores in the slip flow regime, transition regime and molecular regime, in addition to the continuum regime.

The gas flow regimes are classified on the basis of the Knudsen number. For small Knudsen numbers ($Kn < 10^{-3}$), the gas transport in pores is a continuous flow without slip velocity at the wall. When $10^{-3} < Kn < 10^{-1}$, gas can still be considered as a continuous medium, however, gas velocity along the pore wall is not zero any

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Nomenclature

b	the ratio coefficient, fraction
d	pore diameter, m
d_p	methane molecule diameter, m
D	diffusion coefficient, m^2/s
k_B	Boltzmann constant, J/K
k_{app}	the total apparent permeability, m^2
k_{bulk}	the bulk diffusion apparent permeability, m^2
k_K	the Knudsen diffusion apparent permeability, m^2
Kn	Knudsen number, fraction
$\dot{m}^D$	net mass flux induced due to molecular self-diffusion, $kg/(m^2\ s)$
M	gas molar mass, kg/mol
$\dot{M}^C$	mass transport rate for continuum regime, kg/s
$\dot{M}^D$	bulk diffusion mass flux rate, kg/s
$\dot{M}^e$	effective diffusion mass flux rate, kg/s
$\dot{M}^{D*}$	normalized bulk diffusion mass flux rate, fraction
$\dot{M}^{e*}$	normalized effective mass flux rate, fraction
$\dot{M}^{K*}$	normalized Knudsen diffusion mass flux rate, fraction
$\dot{M}^K$	Knudsen diffusion mass flux rate, kg/s
$\dot{M}^T$	total mass flux rate, kg/s
p	pressure, Pa
r	pore radius, m
R	universal gas constant, J/mol/K
T	temperature, K
$\bar{u}^M$	the molecular mean velocity, m/s
λ	the mean molecular free path, m
ρ	density, kg/m^3

more. Hence, this flow regime is called slip flow regime. When $10^{-1} < Kn < 10$, the mean free path λ and pore diameter d are of the same order of magnitude, and both bulk and Knudsen diffusion are equally relevant, which is called transition regime. When $Kn > 10$, few gas molecules collide with each other compared to the number of collisions between molecules and the pore wall. Knudsen diffusion is the most important gas transport mechanism in this regime [3,20]. The conventional approach, based on Darcy's law, captures the continuum flow regime rather well, but is inadequate to describe other flow regimes. Therefore, there is a need to develop a unified transport model to describe shale gas flow in nano-pores under the above mentioned flow regimes.

Two basic approaches exist for describing gas flow in nano-pores: (a) the molecular models, which consider the molecular nature of the gas and (b) the continuum models, which focus on the temporal and special variation of the macroscopic properties of the gas [3]. The molecular models include the Lattice Boltzmann method, the *DSMC* method and the molecular dynamic simulation [4]. Gas flow for high Knudsen numbers ranging in nano-pores can be accurately modeled using molecular models, because the position, velocity and state of all molecules are calculated explicitly at all times [5–9]. The most significant limitation of molecular models is the large computational time and the memory that they require [10].

Continuum models, like Navier–Stokes (*NS*) equations and Burnett equations, can be solved fairly easily under some simplified assumptions. But *NS* equations with no-slip boundary condition are not valid for Knudsen numbers greater than 10^{-3} [3]. Therefore, the first-order and second-order slip flow equations, which can address these limitations, are proposed.

Klinkenberg [11] was the first to identify gas slippage by testing the permeability of gases at different pressures. Jones and Owens [12] proposed an empirical static gas-slippage factor after conducting experiments on tight gas play and compared it with the Klinkenberg slippage factor. Florence et al. [13] correlated the Klinkenberg gas slippage factor and developed a general expression for the apparent gas permeability for tight gas reservoirs. Civan [14] correlated the rarefaction coefficient and the Klinkenberg gas slippage factor and studied the effect of intrinsic permeability, porosity and tortuosity on the apparent gas permeability. However, when the Knudsen number is higher than 0.1, Knudsen diffusion becomes increasingly more significant [15]. Moreover, the slip model parameters have to be determined by fitting the experimental data [4]. Hence, the slip model is limited to describe gas flow in nano-pores under various regimes, especially under the transition regime and the molecular regime.

To overcome the limitations of the slip model, many authors tried to build a unified gas transport model for gas flow under various Knudsen numbers. Liu et al. [16] defined a contribution weight based on the ratio of slip area and total area, which is invalid when the Knudsen number is larger than unity. Javadpour [17] incorporated both slippage and Knudsen diffusion with linear additivity and proposed an apparent permeability, which is a function of pressure and temperature. Rahmanian et al. [18] combined the viscous flow and Knudsen diffusion with a weight coefficient adapted from Aguilera's experiment [19]. Shi et al. [20] built a flow-slip diffusion model based on the weighted average of slip flow and Knudsen diffusion. Wu et al. [21] and Zhang et al. [22] coupled slip flow and Knudsen diffusion with weight factors defined as the ratios of the intermolecular collisions and the molecule-wall collisions to the total collisions, respectively. Though various unified gas transport models are proposed, there are still some limitations. Some models contain several empirical coefficients or a variety of coefficients, which should be tested by experiments. Others may contain unreasonable weight coefficients and are not validated by experimental or molecular simulation data.

Recent theoretical studies [23,24] have pointed out the importance of an additional term into the classical Navier–Stokes equations to describe the axial diffusive mass flux, resulting in the so-called Extended Navier–Stokes Equations (*ENSE*). Dongari et al. [25] studied compressible gas flow through a micro-channel and the Knudsen paradox with *ENSE*. Sambasivan [26] derived an analytical solution procedure to describe the velocity distributions in micro-channels based on the *ENSE*. Moreover, a backward facing step flow was chosen as an example to demonstrate the usefulness of *ENSE* in predicting gas flow in micro-channels and capillaries.

In this paper we develop a unified and, yet, simplified model based on the *ENSE* to describe gas flow in nano-pores under various regimes including the continuum regime, the slip flow regime, the transition regime and the molecular regime. The model is validated with *DSMC* results and experimental data, and the appropriate ratio coefficient is obtained. Then, the gas transport mass, contributed by different flow mechanisms with the variety of Knudsen numbers, is analyzed. Finally, the effect of the ratio coefficient, pore size and pressure on the gas flow are discussed using the proposed model.

2. Model

We now present the model for gas transport in nano-pores based on the extended Navier–Stokes equations. In this model,