Journal of Natural Gas Science and Engineering xxx (2016) 1–6

Contents lists available at ScienceDirect

Journal of Natural Gas Science and Engineering

journal homepage: www.elsevier.com/locate/jngse

Klinkenberg slippage effect in the permeability computations of shale gas by the pore-scale simulations

Jun Li [a, *], Abdullah S. Sultan [a, b]

[a] Center for Integrative Petroleum Research, College of Petroleum Engineering and Geosciences, King Fahd University of Petroleum & Minerals, Saudi Arabia
[b] Department of Petroleum Engineering, College of Petroleum Engineering and Geosciences, King Fahd University of Petroleum & Minerals, Saudi Arabia

ARTICLE INFO

Article history:
Received 9 June 2016
Received in revised form
11 July 2016
Accepted 14 July 2016
Available online xxx

Keywords:
Shale gas permeability
High Knudsen number
Klinkenberg slippage effect
Boltzmann equation
Pore-scale simulation
Monte Carlo molecular simulation

ABSTRACT

The prediction of permeability (i.e., apparent permeability) for the shale gas is challenging due to the Klinkenberg slippage effect that depends on the pore size and gas pressure. A recent Monte Carlo molecular simulation method (i.e., DSBGK method) is employed to accurately compute the permeability by the pore-scale simulations at different pressures. The computed results of a benchmark problem proposed here are used to verify the accuracy of the simple Klinkenberg correlation model, which relates the permeability to the intrinsic permeability (i.e., liquid permeability) and pressure. The verification shows that the Klinkenberg correlation model as a data fitting formula is appropriate for the industry applications since the relative error is small in the whole range of the flow regime as long as it has been calibrated for each particular rock sample at the two ends with low and high pressures, respectively, by determining the model parameters using accurate permeability data that can be obtained by the scheme presented herein. This conclusion is consistent with the experimental observations of real rock samples by Klinkenberg as shown in Appendix.

1. Introduction

Productive gas-shale systems consist of four types of porous media: inorganic matrix, organic matrix, natural fractures and hydraulically induced fractures. Numerous organic flakes are sparsely scattered inside the inorganic matter and intersected by natural fractures (Wang et al., 2009). The Knudsen (Kn) number is defined here as the ratio of the molecular mean free path to the representative pore size, where the molecular mean free path increases with the decrease of pressure during the gas production process. The Kn number is usually large in the organic matter due to the nano-pores, which makes the Klinkenberg slippage effect (Klinkenberg, 1941) remarkable and increases the permeability.

The traditional experimental technique to measure the flow rate at steady state is not applicable for the permeability measurement of shale gas because it requires a considerable time and the low flow speed is usually dominated by the noise in the measurements. The current pulse-decay approach measures the pressure evolutions at the two ends of a rock sample, which are then used in a partial differential equation (PDE) to estimate the permeability that is regulated until the computed pressure response at the outlet matches the measured one under the same inlet pressure pulse (Jin et al., 2015). Obviously, this approach is not purely experimental measurements and its validity depends on the accuracy of the PDE used.

Gas flow problems at different scales need different theoretical descriptions. If the pore size is comparable to the molecular mean free path but much larger than the molecular size of the fluid, the flow phenomenon and the boundary condition can be described by statistical models. Deterministic models, like molecular dynamics (MD) simulation, become necessary only if the pore size is comparable to the molecular size of the fluid. In the case of shale gas, the pores with a size comparable to a methane molecule are usually blocked due to adsorption and so negligible in the computation of permeability. Thus, the statistical models are valid to simulate the pore-scale flows of shale gas. The gas flows can be divided into different regimes according to Kn (Shen, 2005; Freeman et al., 2011): 1) continuum regime with $Kn < 0.01$ (*note*: not 0.001 as shown in the following results), where the Navier-Stokes (N–S) equation and the no-slip boundary condition are valid; 2) slip regime with $0.01 < Kn < 0.1$, where a slip boundary condition should be used with the N–S equation; 3) transitional regime

* Corresponding author.
E-mail addresses: lijun04@gmail.com (J. Li), sultanas@kfupm.edu.sa (A.S. Sultan).

http://dx.doi.org/10.1016/j.jngse.2016.07.041
1875-5100/

$0.1 < Kn < 10$, where the Boltzmann equation at the molecular level in a statistical way is necessary; 4) free molecular flow regime $10 < Kn$, where the Boltzmann equation is significantly simplified and analytical solutions are sometimes available. The operating range of productive shale gas usually covers the slip and transitional regimes (Freeman et al., 2011). Compared to the pore-scale gas flows in the conventional reservoir with large pore size and thus small *Kn*, the adsorption and slippage effects at the pore surface are remarkable in the shale gas flows due to small pore size. The adsorption effect is neglected here and the current study focuses on the permeability variation with pressure due to the Klinkenberg slippage effect. The adsorption effect can be reflected by modifying the pore space according to the adsorption thickness at the pressure concerned (Sakhaee-Pour and Bryant, 2012), which will be investigated in future work.

Many empirical correlation models are proposed to estimate the permeability variation with pressure for shale gas as discussed in (Chen et al., 2015). Klinkenberg first proposed a simple and first-order model, which was obtained using the N–S equation with slip boundary condition in the unidirectional channel flow problems but also applied as a data fitting formula to analyze the experimental permeability data of real rock samples at high *Kn* (Klinkenberg, 1941). A second-order correlation is proposed (Beskok and Karniadakis, 1999) and the coefficient can be correspondingly determined (Civan, 2010). Additionally, the dusty gas model (DGM) can be used to derive a different estimation model, which correlates the permeability to the intrinsic permeability, effective diffusivity, viscosity and pressure (Sakhaee-Pour and Bryant, 2012; Ho and Webb, 2006), and the coefficients are determined for real rock samples in (Chen et al., 2015). These correlation models for the estimation of permeability are proposed to avoid the pore-scale simulations of the gas flows at high *Kn*, which require sophisticated computational methods based on the complicated integro-differential Boltzmann equation.

The permeability variation with pressure is numerically studied here by the pore-scale simulations of gas flows using a recent Monte Carlo molecular simulation method, namely the DSBGK method (Li, 2010, 2012a,b) based on the Bhatnager-Gross-Krook (BGK) equation that is a good approximation to the Boltzmann equation in rarefied gas problems with small perturbations and accurate at high pressures (at least up to 3 MPa in the current study with comparison against the LBM result as a criteria at high pressure). The DSBGK method is verified against the standard direct simulation Monte Carlo (DSMC) method (Bird, 1963, 1994) over a wide range of *Kn* number in several benchmark problems but much more efficient than the DSMC method. To make the results reproducible and available for the verifications of other numerical methods, a two-dimensional benchmark problem is proposed here to study the Klinkenberg slippage phenomenon. The computed results for real three-dimensional digital rock samples with 100-cubed voxels over a wide range of *Kn* are given in (Li and Sultan, 2015). To the best of our knowledge, the present work is the first study that investigates the Klinkenberg slippage effect in the apparent permeability using accurate pore-scale simulations rather than correlation models.

For the pore-scale simulations, the traditional DSMC method is a standard method to obtain solutions of the Boltzmann equation at arbitrary *Kn* but its computational cost is prohibitive in the case of low-speed as occurred in the shale gas because of statistical noise (Shen, 2005). The ordinary lattice Boltzmann method (LBM) applies a very rough discretization in the molecular velocity space to solve the BGK equation and its accuracy at large *Kn* can be improved by increasing the number of velocity points, which unfortunately will increase the computational cost significantly (Watari, 2010). A simple but artificial scheme is to modify the effective viscosity by adjusting the relaxation time but the verifications are usually limited to unidirectional flows in a moderate range of *Kn* (Zhang et al., 2005; Guo et al., 2008; Zhang et al., 2014).

2. Simulation method

The pore-scale gas flows at different pressure conditions are simulated here by the Fortran MPI software package NanoGasSim developed using the DSBGK method that is detailed in (Li, 2012a). At the initial state, the computational domain is uniformly divided into many cells, which are either void or solid, and about twenty simulated molecules are randomly distributed inside each void cell (i.e., pore space) and assigned with the initial positions, velocities and other molecular variables according to a specified initial probability distribution. Each simulated molecule moves uniformly and in a straight line before randomly reflecting at the surfaces of solid cells according to the diffuse reflection model that is accurate for usual surfaces without polishing, including both organic and inorganic surfaces inside the shale rocks. During each time step, the trajectory of each particular molecule may be divided into several segments by the cell's interfaces and its molecular variables are updated along each segment in sequence at the moving direction. Simulated molecules are removed when moving across the open boundaries during each time step and then new simulated molecules are generated after each time step at the open boundaries according to the specified pressures as in the DSMC simulations. At the end of each time step, the number density, flow velocity and temperature at each void cell are updated using the increments of molecular variables along these segments located inside the concerned cell according to the conservation laws of mass, momentum and energy of the intermolecular collision processes. For each simulation at a given pressure, the volumetric velocity component along the driving direction at steady state is used to compute the permeability.

Although the algorithm of DSBGK method is similar to that of the traditional DSMC method, there are obvious differences between them: 1) the DSMC method uses the transient values of molecular variables to compute the cell's variables while the DSBGK method employs the increments rather than the transient information of molecular variables to update the cell's variables based on the mass, momentum and energy conservation principles of intermolecular collision process occurred within each cell; 2) the DSBGK method computes the effect of intermolecular collisions by solving the BGK model while the DSMC method handles the collision effect by randomly sampling. This two differences lead to significant improvement of efficiency in the DSBGK simulations at low speed by reducing stochastic noise. More discussions are detailed in (Li, 2012a).

3. Results and discussions

A two-dimensional benchmark problem is proposed in Fig. 1, where the definition of the representative pore size R is clear. The domain sizes at both x and y directions are the same and equal to $L = 5R$. The computational domain is divided into many cells and we use ΔL to denote the cell size if $\Delta x = \Delta y$ while sometimes $\Delta x \neq \Delta y$ is applied to investigate the influences of spatial resolution at different directions to the simulation accuracy. The time step Δt is selected to make the average molecular displacement during each Δt is smaller than the molecular mean free path λ_0. The pressure difference between the inlet and outlet is only 1% here such that the dependence of permeability on the pressure can be accurately studied. For each simulation at a given pressure p_0, the volumetric velocity component $\overline{u}$ along the driving direction at steady state is used to compute the permeability κ as follows:

Please cite this article in press as: Li, J., Sultan, A.S., Klinkenberg slippage effect in the permeability computations of shale gas by the pore-scale simulations, Journal of Natural Gas Science and Engineering (2016), http://dx.doi.org/10.1016/j.jngse.2016.07.041