



# Numerical and experimental study on gas flow in nanoporous media



Zhengyi Li <sup>a</sup>, Chenji Wei <sup>b</sup>, Juliana Leung <sup>c</sup>, Yuhe Wang <sup>d</sup>, Hongqing Song <sup>a,\*</sup>

<sup>a</sup> School of Civil and Environmental Engineering, University of Science and Technology Beijing, China

<sup>b</sup> Research Institute of Petroleum Exploration and Development, PetroChina, China

<sup>c</sup> Department of Civil and Environmental Engineering, University of Alberta, Canada

<sup>d</sup> Department of Petroleum Engineering, Texas A&M University at Qatar, Qatar

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## ABSTRACT

With the increasing attention being paid to the development of unconventional reservoirs, such as shale gas or tight gas reservoirs with nanoscale pores, over the last few years, there is a great demand to develop a coherent theoretical framework that explains the transport mechanisms that take place in a nanoporous medium. In this paper, a complete modelling workflow that spans the mesoscale to the macroscale, including the lattice Boltzmann model (LBM) and Navier–Stokes equations, is introduced to reflect these transport characteristics. Gas flow for different pore diameters and Knudsen numbers is simulated by LBM. Comparison between physical experimental measurements and the LBM simulation results shows that the general transport equation is most appropriate for describing gas flow in nanoporous media and that the values of the diffusion coefficient and intrinsic permeability can be obtained simultaneously using this equation. Intrinsic permeability decreases faster than the diffusion coefficient with the decreasing average pore diameters in nanoporous media. The general transport equation has been verified to reflect the mechanisms of flow and diffusion in nanoporous media, and it also provides a theoretical basis to assess the results attained from numerical simulations.

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## 1. Introduction

The slippage effect is often invoked to explain the difference between gas flow and liquid flow in a porous medium. Klinkenberg concluded from a series of gas flowing experiments that gas permeability varies with the average pressure. An equation was subsequently presented to describe the gas permeability variation with pressure; however, it is applicable for only certain flow regimes and is not valid for flow in a nanoporous medium (Klinkenberg, 1941). The Knudsen number ( $Kn$ ) is a measure for classifying different states of sparse gas flow in pores. The regime of gas flow is divided into four types: Knudsen flow ( $Kn > 10$ ), transition flow ( $0.1 < Kn < 10$ ), slip flow ( $0.01 < Kn < 0.1$ ) and continuum flow ( $Kn < 0.01$ ) (Xiao and Wei, 1992). For gas flow in nanoporous media, the collisions of gas molecules dominate because the pore diameters are too narrow. The Dusty-Gas model (DGM) is a multicomponent convective and diffusive theory that is valid for all gas flowing regimes (Thorstenson and Pollock, 1989; Freeman et al., 2011). After DGM is introduced to modify the slip factor, the

Klinkenberg equation can be revised to a new general equation (Song et al., 2013). The new general transport equation can incorporate various transport mechanisms that take place in a nanoporous medium, including convection and diffusion. However, there is no coherent theoretical framework to explain this equation or to simultaneously obtain the values of permeability and the diffusion coefficient with this equation.

Numerical simulation is a commonly-adopted method of studying flow mechanisms, and the simulation results are stable and credible. However, traditional simulation may not be appropriate for modelling gas flow in nanoporous media without considering the meso/microscale effects, which include slippage, transition flow and Knudsen diffusion. The Lattice Boltzmann method (LBM) is a type of numerical simulation method that is capable of modelling this meso/microscale fluid system (Guo and Zhao, 2002). Previous LBM simulation studies have employed different modified equations of the slippage effect to describe the gas transport mechanism; hence, these simulations could result in misleading interpretations due to ignoring the micro-structure of nanoporous media (Chen et al., 2008; Li and Yu, 2011).

A physical experiment is an efficient and authoritative method to research and demonstrate gas transport characteristics. Shale gas

\* Corresponding author.

E-mail address: [songhongqing@ustb.edu.cn](mailto:songhongqing@ustb.edu.cn) (H. Song).

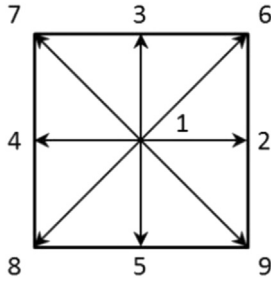


Fig. 1. Distribution of the velocities in the D2Q9 model.

transport in porous media can be explained by the theory of gas flow in nanoporous media. The results from physics experiments reflected the impact of the diffusion coefficient and permeability of a nanoporous medium (Song et al., 2014; Wan et al., 2015). However, the materials and labour costs of traditional physical experiments are high, and the process is often difficult and time-consuming. Moreover, the relationship between gas transport and the diameter of the pores cannot be determined via a traditional physical experiment (Song et al., 2015; Huang et al., 2015). A proper numerical simulation, such as LBM, can explain these relationships.

In this paper, a complete modelling framework that spans the mesoscale to the macroscale, including the lattice Boltzmann model and Navier–Stokes (N–S) equations, is introduced to reflect the transport characteristics in nanoporous media. Physical experiments are conducted to quantify the transport characteristic of gas flow in nanoporous media. Gas flow in media characterized by different pore diameters and Knudsen numbers is simulated using LBM. The diffusion coefficient and permeability can be calculated from the experimental results and compared with the numerical results obtained from LBM. The comparison illustrates the capability of LBM to simulate gas flow in nanoporous media. The results calculated by using the traditional gas slip equation, Darcy equation and general transport equation (Song et al., 2013) are subsequently compared with the simulation results of LBM. Based on the theoretical framework of LBM, the results show good agreement with the general transport equation, which is the best model for gas flow in nanoporous media.

## 2. Mathematical model

### 2.1. Gas flow in nanoporous media

The N–S equation describes the dynamic characteristics of viscous flow and includes the components of body force, viscous force and pressure. Gas flow in a porous medium is a type of low-speed flow; thus, the compressibility of the gas can be ignored and the density is considered to be a constant value. The incompressible N–S equation can be expressed as (Nithiarasu et al., 1997):

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla \cdot (p\delta) = -\mu \nabla^2 \mathbf{u} + \rho \mathbf{g} \quad (1)$$

where  $\mathbf{u}$  is the flowing velocity,  $\rho$  is the density,  $t$  is the time,  $p$  is the pressure,  $\delta$  is a tensor with a value of  $\delta_{ij}$ ,  $\mu$  is the viscosity, and  $\mathbf{g}$  is the gravity. For fluid dynamics in porous media, some aspects of the N–S equation should be modified. First,  $\mathbf{u}$  should be replaced by  $\frac{\mathbf{u}}{\phi}$  because the velocities in a porous medium are macroscopic values. Assuming that a statistical average is tenable,  $\nabla^2 \mathbf{u} = \frac{1}{c} \left( \frac{\mathbf{u}}{\bar{d}_{pore}^2} \right)$  (Shen, 2000), where  $\bar{d}_{pore}$  is the average pore diameter,  $c$  is the non-

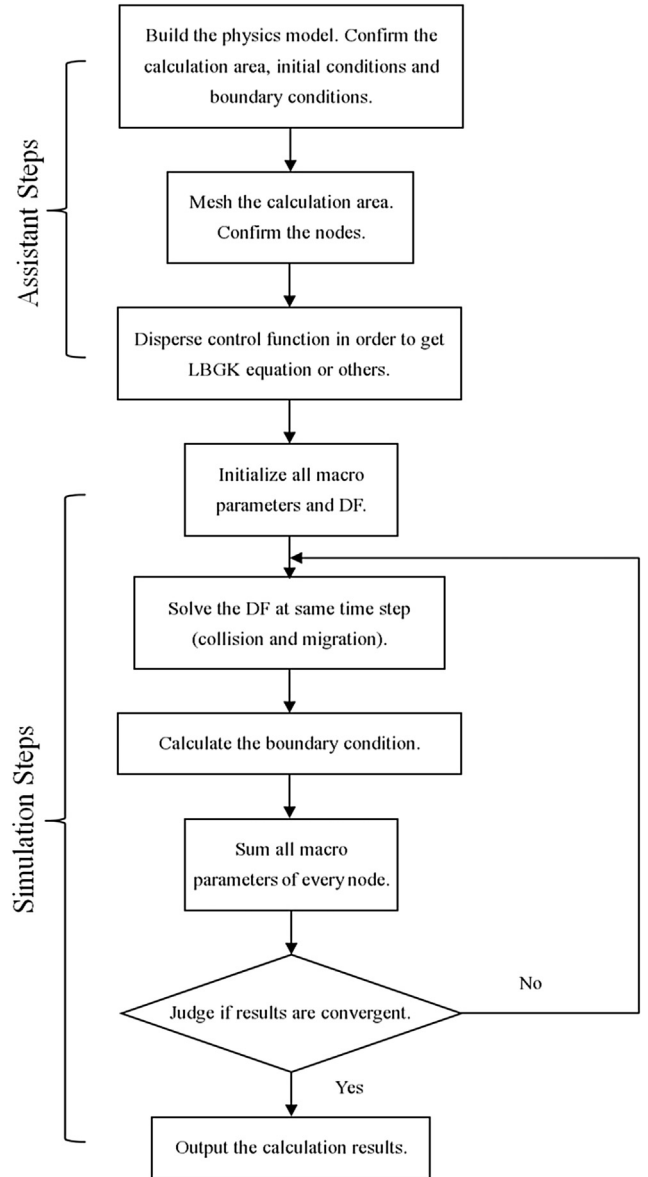


Fig. 2. Basic simulation process with LBM.

dimensionless shape parameter, and the tensor  $\nabla \cdot (p\delta)$  can be simplified to a scalar  $\nabla p$ . Therefore, the Navier–Stokes equation for flow in porous media can be formulated as:

$$\phi^{-1} \rho \frac{\partial \mathbf{u}}{\partial t} + \phi^{-2} \rho(\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla p = -\phi^{-1} \frac{\mu}{c \bar{d}_{pore}^2} \mathbf{u} + \rho \mathbf{g} \quad (2)$$

It is assumed that  $K = c \bar{d}_{pore}^2 \phi$ . When the flowing velocity is stabilized,  $\frac{\partial \mathbf{u}}{\partial t}$ , and the convective acceleration term becomes zero; the N–S equation can then be rewritten as:

$$\mathbf{u} = -\frac{K}{\mu} (\nabla p - \rho \mathbf{g}) \quad (3)$$

Eq. (3) is the Darcy equation, which can express most of the flowing characteristics in a porous medium. In most cases, horizontal flow is investigated and gravity is ignored. For gas flow without considering gravity, the Klinkenberg equation is presented as follows:

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