PS Numerical Modeling of Adsorption and Roughness Effects on Gas Transport in Shale Using the Lattice Boltzmann Method*

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Abstract

Advanced techniques have greatly promoted the exploitation of shale gas from shale matrix with low permeability. But the gas transport mechanism in shale is still unclear. Due to the multi-scale pore systems in a shale reservoir, viscous flow, slip flow, Knudsen diffusion and adsorption/desorption should be applied to the flowing equation so that it can properly predict gas flow dynamics. Multi-scale simulations are performed to investigate the shale transport mechanism in organic matter by LBM.

Firstly, a generalized model with roughness surface was proposed to investigate the competitive effects of gas slippage, roughness surface and adsorption layer on permeability of shale matrix. A pressure-dependent adsorption thickness and relative roughness were adopted in the present study. Then a multiple-scale integration method was proposed to upscale the pore-scale simulations to field-scale problems. Decline curve analysis was studied to predict the production of shale gas. The results showed that the surface roughness has remarkable effects on gas flow. The streamlines near rough surface are distorted and the axial velocity is strengthened. This is because gas molecular and rough surface is undergoing multi-collisions under roughness diastema region. Shale tends to adsorb on the organic matter surface, so the roughness surface also affects the adsorption. Adsorbed layer affects the gas flow in organic matters through two ways: reducing the volume of void space and changing the slippage. The existence of adsorption will reduce the actual pore size and the higher the pressure, the lower the actual pore size. The positive effect of slippage overwhelms the negative effect of adsorption. Under lower pressure, slippage is stronger and the volume of adsorption is less, leading to higher apparent permeability than intrinsic permeability. In DCA, the rarefaction effect is found to be dominant at the early stage while the compressibility effect becomes dominant at late stage, which results in respectively an overestimation and an underestimation of the gas production. The permeability estimation is also be compared with the experimental data and a good match is achieved. This article adopted a pressure-dependent adsorption thickness and a novel boundary scheme, and reduces the mass flux error near the solid surface, to conduct further studies of the microcosmic transport mechanism.

Numerical Modeling of Adsorption and Rough Effects on Gas Transport in Shale Using the Lattice Boltzmann Method

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Abstract

Over the past decades, advanced techniques have greatly promoted the exploitation of shale gas from shale matrix with low permeability. The gas transport mechanism in shale is still unclear on one hand and on the other hand roughness surface and adsorbed layer have significant impact on the apparent permeability of shale gas flow. However, studies on the effect of the roughness surface and adsorbed layer on the productivity are rare, partly because of the difficulty in linking the results of pore scale and field scale.

The objective is to propose a method to simulate gas flow through nanometer channels with roughness surface and investigate the effect of roughness and adsorption on the apparent permeability, and further study its effect on the productivity. In this study, we combined dust gas model (DGM) and generalized Maxwell-Stefan model (GMS) to calculate the apparent permeability considering viscous flow, Knudsen diffusion, surface diffusion and desorption, and introduced these into lattice Boltzmann model with roughness surface. Fractal geometry was introduced to model the surface roughness, and the roughness was characterized by two parameters, i.e., relative roughness height and fractal dimension. Afterwards, a pressure-dependent adsorption thickness was adopted to study the effect of pore size change. The above mechanisms were applied to study the overall effects on apparent permeability by simulating flow in a reconstructed 2D porous media. Finally, the apparent permeability was propagated to the calculating of productivity through iteration step, and micro-scale effect on productivity was analyzed.

Introduction

To be specific, 20%~80% of shale gas exists in the adsorbed state on the surface of organic particulates. Thus, the seepage of shale gas reservoirs have specific adsorption/desorption and diffusion characteristics. Adsorption occurs on the solid surface and generates adsorbed layer. The adsorbed layer not only changes the interactions between gas molecules and the wall, but also occupies a significant part of the void space of a nanometer channel. Even though the existing researches can already represent the main seepage characteristics of shale gas reservoirs, they usually fail to comprehensively consider the micro-scale seepage and the desorption effect. And present researches consider the adsorbed layer has a constant thickness, but actually the adsorption thickness is pressure-dependent.

Shale gas flows in nanometer channels with Knudsen number from 0.006 to 0.8.The roughness surface has significant impact on the apparent permeability especially when the Knudsen is larger than 0.1. Several numerical methods have been utilized to study the effect of roughness surface on shale gas flows in nanometer channels. But most existing studies are based on the slip flow with low Knudsen number. Another major problem among the previous studies is the quantitative characterization of surface topography. In most of the studies, a statistical average roughness height is used to describe the surface topography. But, experimental results show that the roughness surface is a nonstationary random process for which the roughness height distribution is related with the measuring resolution and sample length.

One challenge for pore-scale modeling of shale gas is the multiscale issue. The target is to understand and predict the production at field scale. However based on the computational cost, the pore-scale simulation is usually limited to very small volume. An efficient upscaling method is desperately desired to bridge the microscale simulation results and the macroscale prediction.

1. Apparent permeability prediction of organic shale considering surface diffusion effect

1) Methodology

a) Dusty gas model

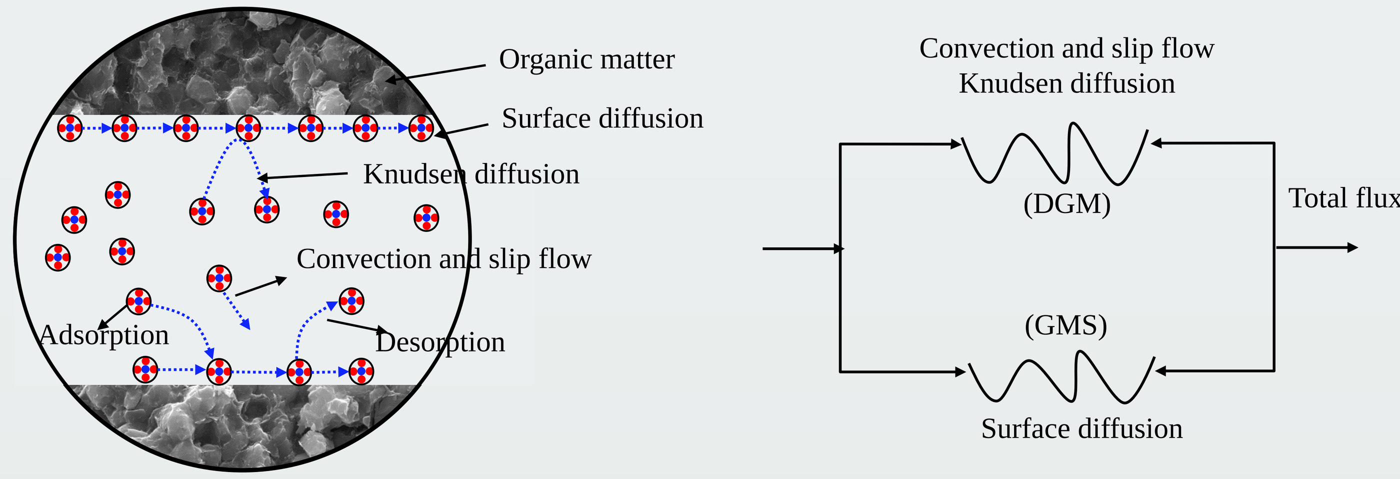
The DGM is based on the combination of the Maxwell-Stefan diffusion equations and the characteristics of mass transfer in porous media. The basic idea of DGM is to consider the solid as a dummy species of infinite mass, which is constrained by unspecified external forces and has zero drift velocity. If the system contains only one species, the flux equation of the DGM holds:

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

b) 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. Assuming that the Langmuir equation to be valid and the adsorption equilibrium to be established, the surface diffusion flux in terms of partial gradient satisfies:

$$N_{GMS} = (1-\varepsilon)q_{sat}\frac{bD_s}{1+bP}\frac{\partial P}{\partial r}$$



c) Apparent permeability prediction

For a single gas species the combination of the DGM and the GMS results in the total flux:

$$N_{total} = -\left(\frac{1}{RT}\left(D_K + \frac{K_0}{\eta}P\right) + (1-\varepsilon)q_{sat}\frac{bD_s}{1+bP}\right)\frac{\partial P}{\partial r}$$

As the surface diffusion of adsorbed gas only happens in organic matter, the apparent permeability of inorganic matter is:

$$K_{app,iom} = \frac{\eta M}{\rho_g}\left(\frac{1}{RT}\left(D_K + \frac{K_{0,iom}}{\eta}P\right)\right)$$

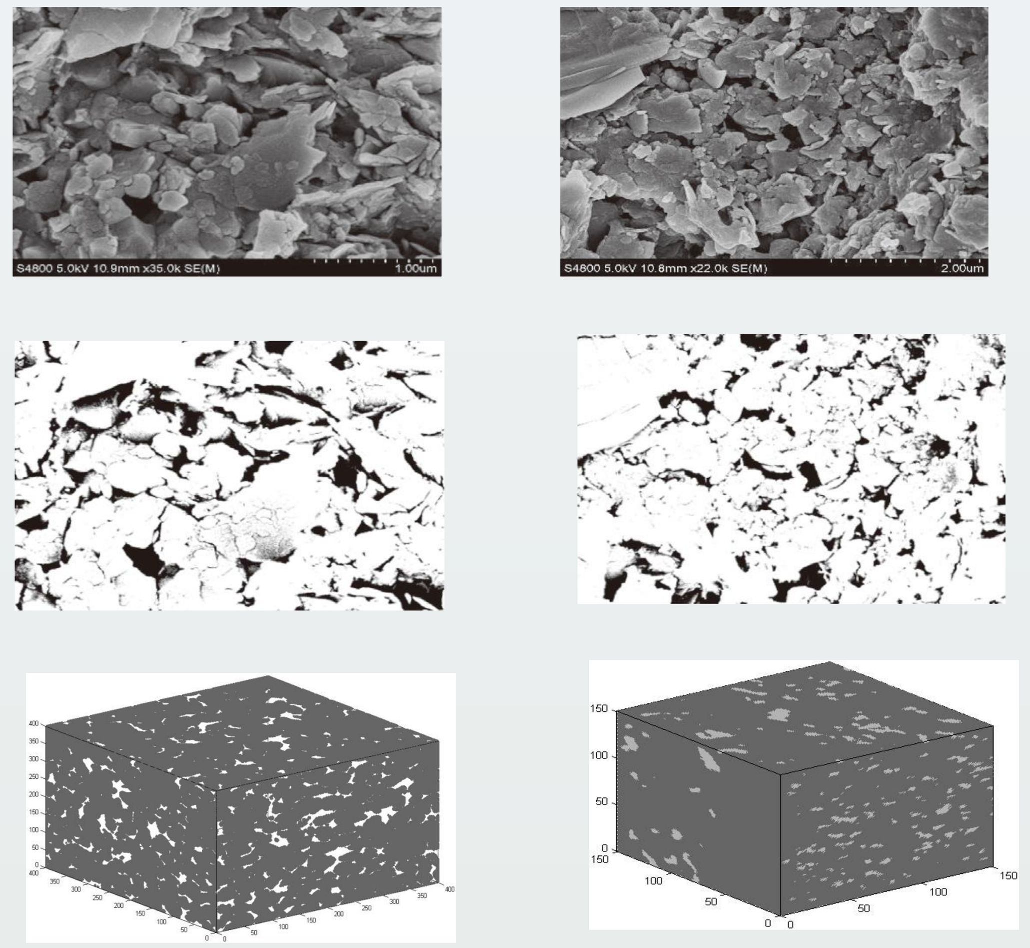
And, the apparent permeability of organic matter is:

$$K_{app,om} = \frac{\eta M}{\rho_g}\left(\frac{1}{RT}\left(D_K + \frac{K_{0,om}}{\eta}P\right) + (1-\varepsilon)q_{sat}\frac{bD_s}{1+bP}\right)$$

2) 3D porous media

a) Reconstruction method

- Collect either 2D images of the sample`s pore structure by SEM or 3D images of pores structures by FIB-SEM and Nano/Micro CT. The original SEM gray image should be transformed into a binary image by an iterative threshold method. After alleviating noise of the image by non-local means algorithm, we use Otsu algorithm to segment the images and obtain the binary images.
- Construct the 3D digital rock model from the pore structure images. The digital rock model is built from the 2D SEM images by numerical reconstructed method. In this work the simulated annealing and Gaussian simulation method are used to reconstruct the 3D digital rock of shale.



b) Expectation-Maximization algorithm

Current nitrogen adsorption tests indicate that the pore size distributions in shale usually satisfy double-mode distributions and the assumption of Gaussian distribution for probability distribution function of pore size in rocks has been reported in several studies.

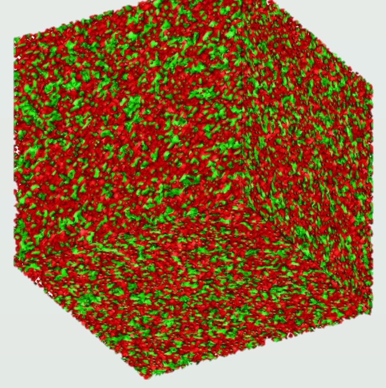
Expectation step

$$w_j^i = \frac{g_j(x)\Phi_j}{\sum_{l=1}^{k} g_l(x)\Phi_l}$$

Maximization step

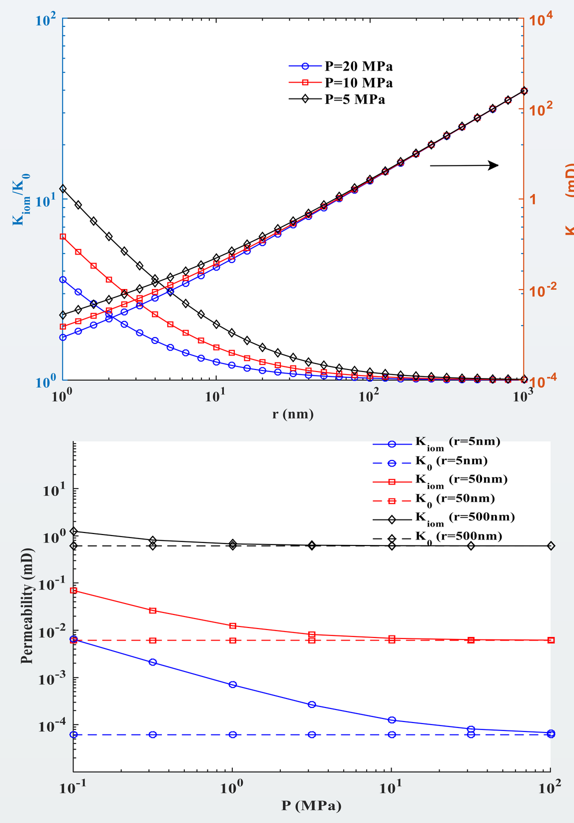
$$\Phi_j^{(new)} = \frac{1}{m}\sum_{i=1}^{m} w_j^i$$

$$\sum_j^{(new)} = \frac{\sum_{i=1}^{m} w_j^{(i)}\left(x^{(i)}-\mu_j\right)\left(x^{(i)}-\mu_j\right)^T}{\sum_{i=1}^{m} w_j^{(i)}}$$

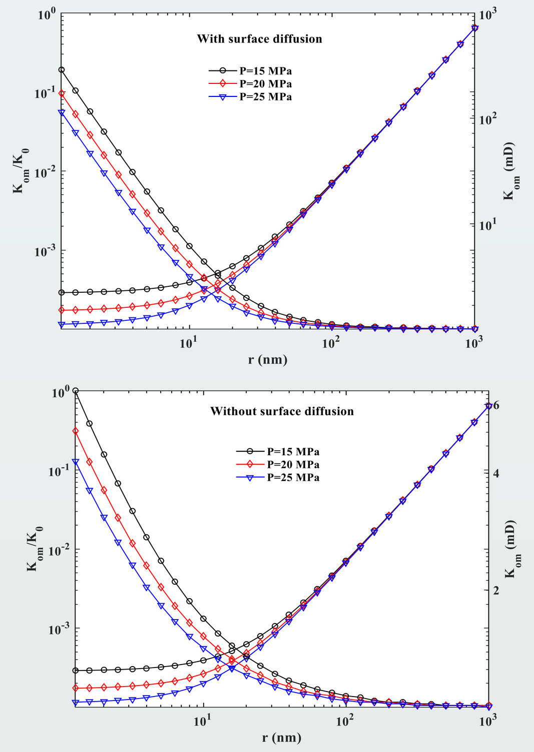


3) Permeability of IOM and OM

a) Permeability of IOM

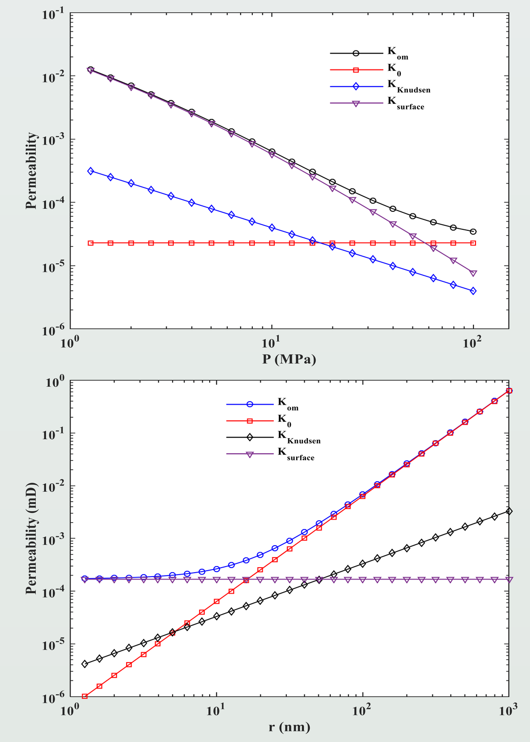


- With the increase of the mean pore radius, K_{iom} increase, so dose its rate of change. K_{iom}/K_0 and its slope, however, decrease with the increase of mean pore radius. When the mean pore radius approaches 100nm, the gas flow becomes continuum, and K_{iom} approximately equals K_0. The permeability of IOM in shale will be underestimated if the Knudsen diffusion is ignored.
- As the average pressure increases, the intrinsic permeability does not change, but K_{iom} decrease. The permeability of IOM is a function of reservoir pressure, and the permeability must be considered as a dynamic reservoir parameter and updated accordingly as the reservoir is being depleted.



b) Permeability of OM

- The trend of K_{om}/K_0 and K_{om} is similar to that of IOM. In large pores, both Knudsen diffusion and surface diffusion can be ignored, and K_{om} is equals to K_{iom}.
- The surface diffusion is the primary flow mechanism in nano-pores, and significant underestimation of permeability can be observed if the surface diffusion is ignored when the average pore radius is less than 10nm.



- The surface diffusion decreases linearly with the increasing pressure, and the contribution from both Knudsen diffusion and surface diffusion becomes almost negligible when the pressure reaches a high level.
- The surface diffusion is the dominant mass transport mechanism in OM at low pressures, and K_{om} accounting for surface diffusion can be several times larger than that without considering it.

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2. Shale flow through rough microchannel

1) Methodology

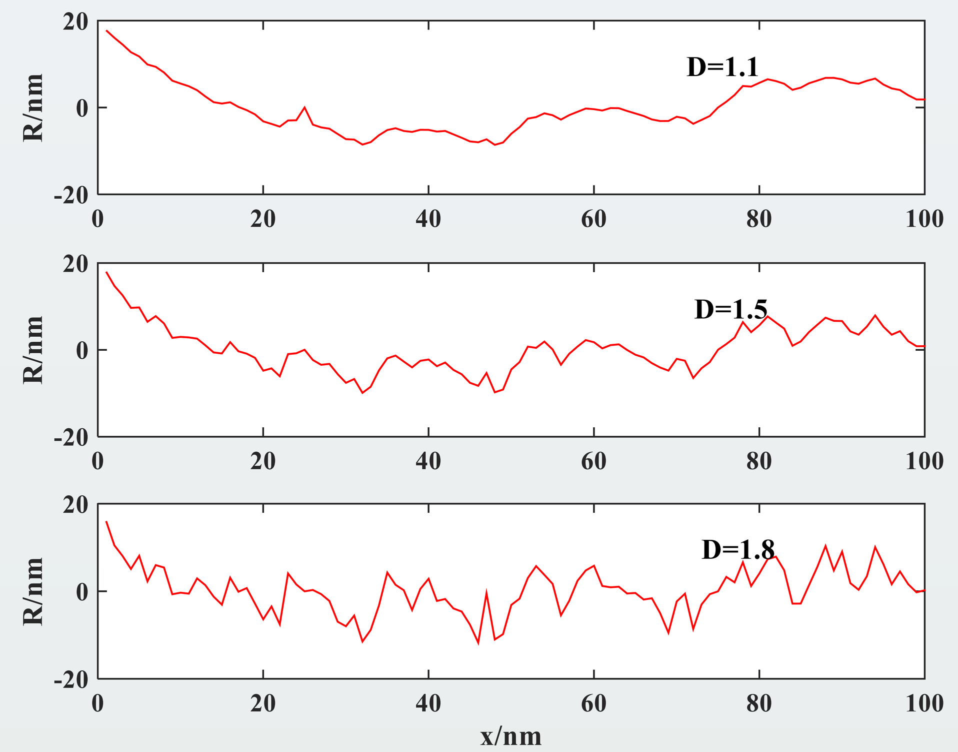
a) Fractal surface

The quantitative characterization of surface topography is the premise to investigate the roughness effect on gas flow in microchannels. The self-affine and multiscale properties of the rough surface profile are satisfied by the Meierstrass-Mandelbrot fractal function.

$$R(x)=G^{(D-1)}\sum_{n=n_1}^{\infty}\frac{\cos\left(2\pi\gamma^{n}x\right)}{\gamma^{(2-D)n}}$$

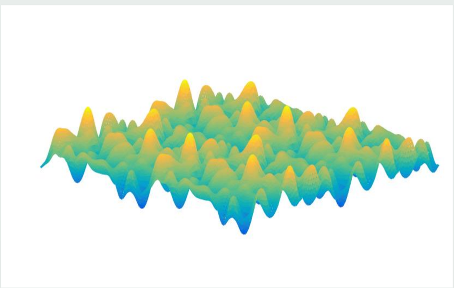
The root mean square roughness height is

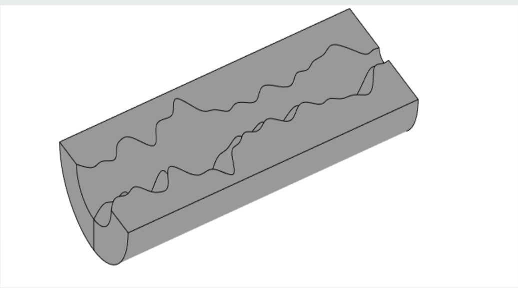
$$\sigma=\left[\frac{G^{2(D-1)}}{2\ln\gamma}\frac{1}{4-2D}\left(\frac{1}{\omega_l^{(4-2D)}}-\frac{1}{\omega_h^{(4-2D)}}\right)\right]^{0.5}$$

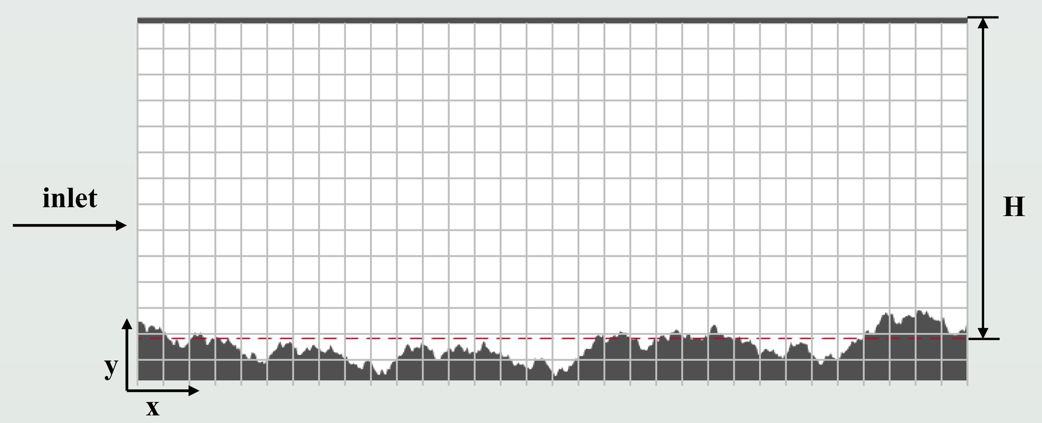


b) Mathematical model

2D and 3D model with roughness surface, characterized by the W-M function and Gaussian equation, were proposed and analyzed numerically.

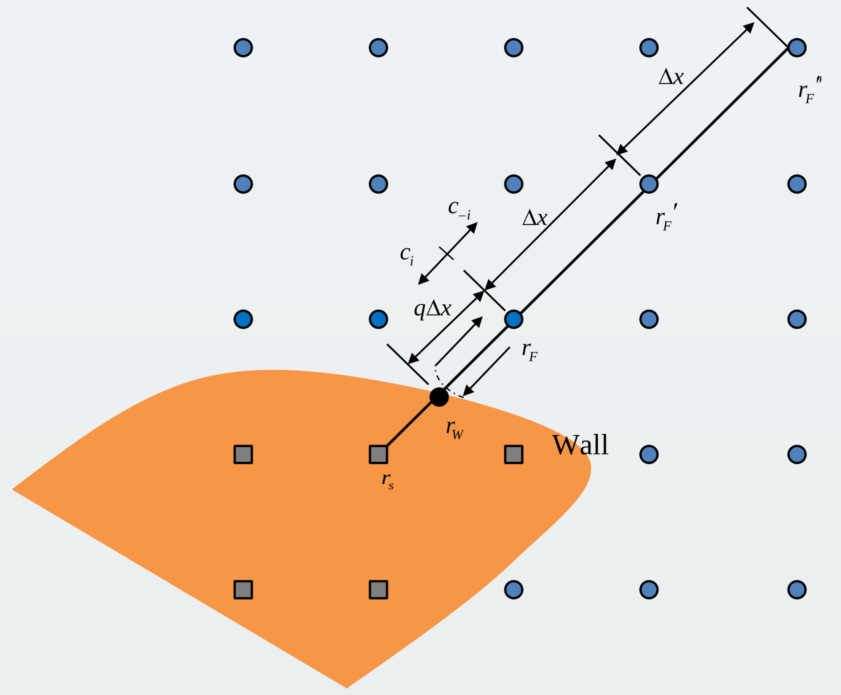






c) Lattice Boltzmann model

- LB simulations generally apply one of the interpolation-based schemes when treating boundaries with complex geometries arbitrary curvatures. Interpolation is performed only near the boundary nodes rather than throughout the entire computational domain based on the uniform mesh defined on Cartesian coordinate.
- For a rigid wall with no-slip condition, the bounce-back boundary treatment is the most easily implemented scheme. Treating curved boundaries by combining the bounce-back scheme with an interpolation approach.



When linear interpolation is applied, the model can be formulated as:

$$f_{-i}\left(\mathbf{r_W},t+\delta_t\right)=\frac{q(1+q)}{2}f_i\left(\mathbf{r_S},t+\delta_t\right)+\left(1-q^2\right)f_i\left(\mathbf{r_F},t+\delta_t\right)-\frac{q(1-q)}{2}f_i\left(\mathbf{r_F}',t+\delta t\right)$$

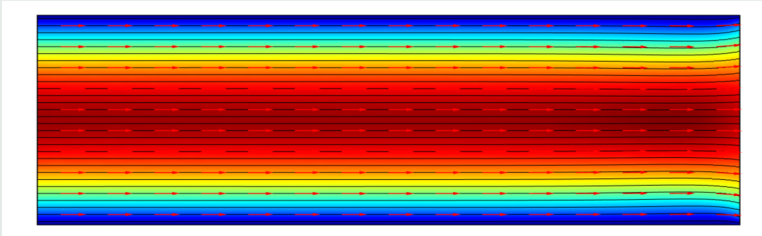
When quadratic interpolation is applied, the model can be formulated as:

$$f_{-i}\left(\mathbf{r_S},t+\delta_t\right)=\frac{1}{(2+q)(1+q)}[q(1+q)f_i'\left(\mathbf{r_F},t\right)+2\left(1-q^2\right)f_i'\left(\mathbf{r_F}',t\right)-q(1-q)f_i'\left(\mathbf{r_F}'',t\right)$$
$$+2q(2+q)f_{-i}'\left(\mathbf{r_F},t\right)-q(1+q)f_{-i}'\left(\mathbf{r_F}',t\right)]$$

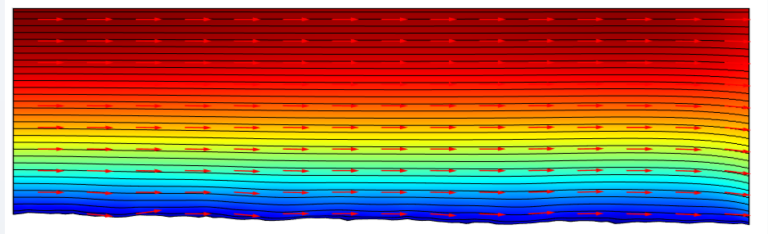
2) Flow simulation

a) Velocity distribution

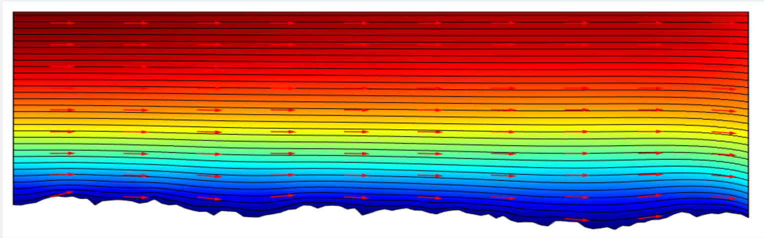
- The existence of surface roughness obviously disturbs the velocity distribution across the microchannel.
- The whole velocity level along the streamwise direction in smooth microchannel is larger than that in rough microchannel.
- The presence of roughness suppresses the velocity slip at the boundary and contributes to extra energy loss in comparison to a smooth surface.



smooth

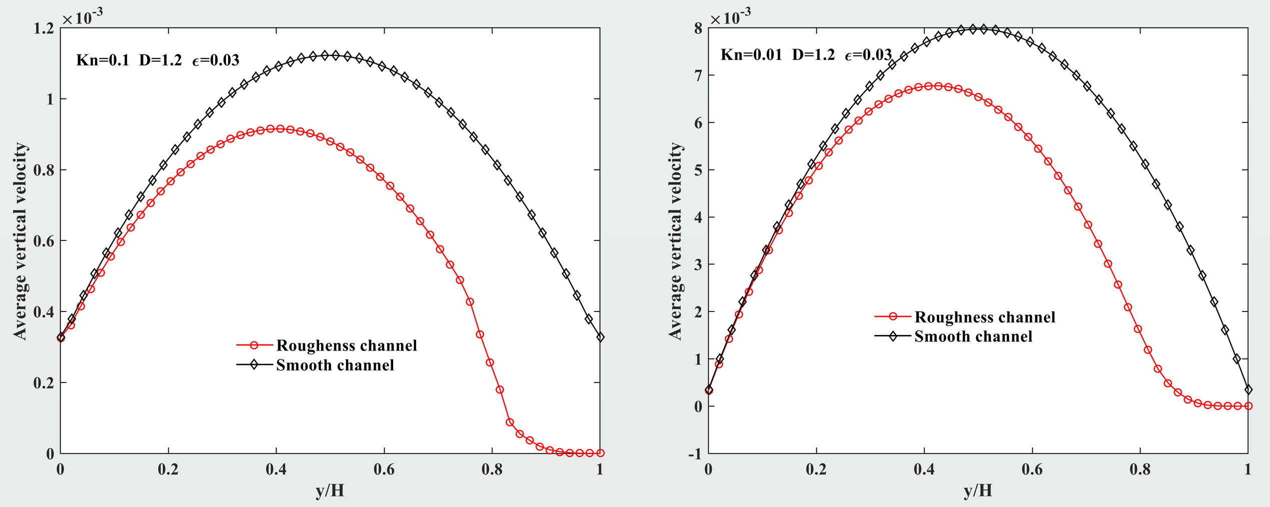


ε=2%

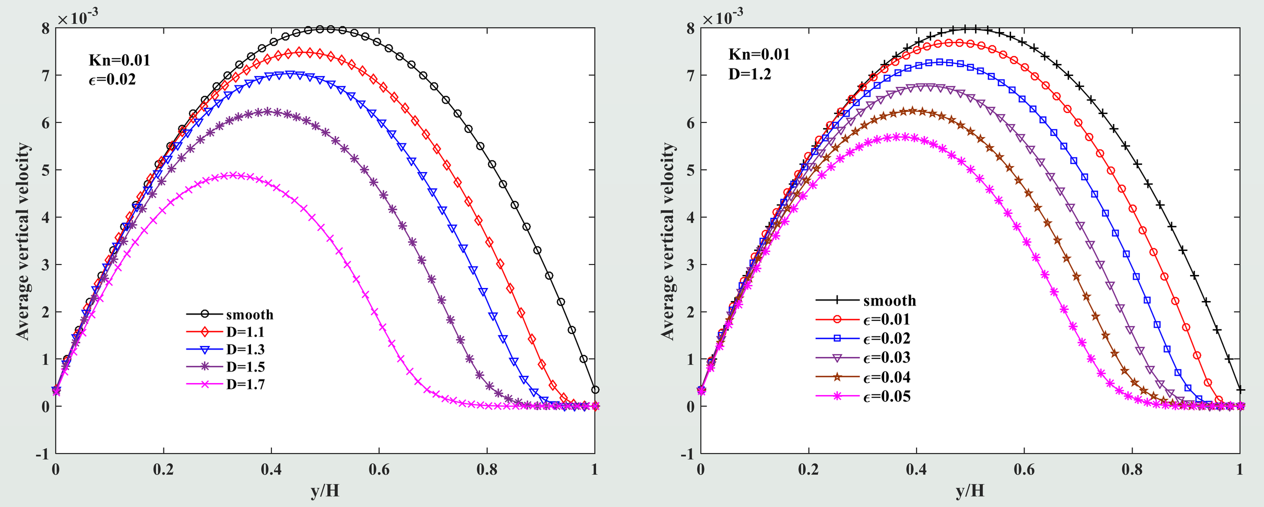


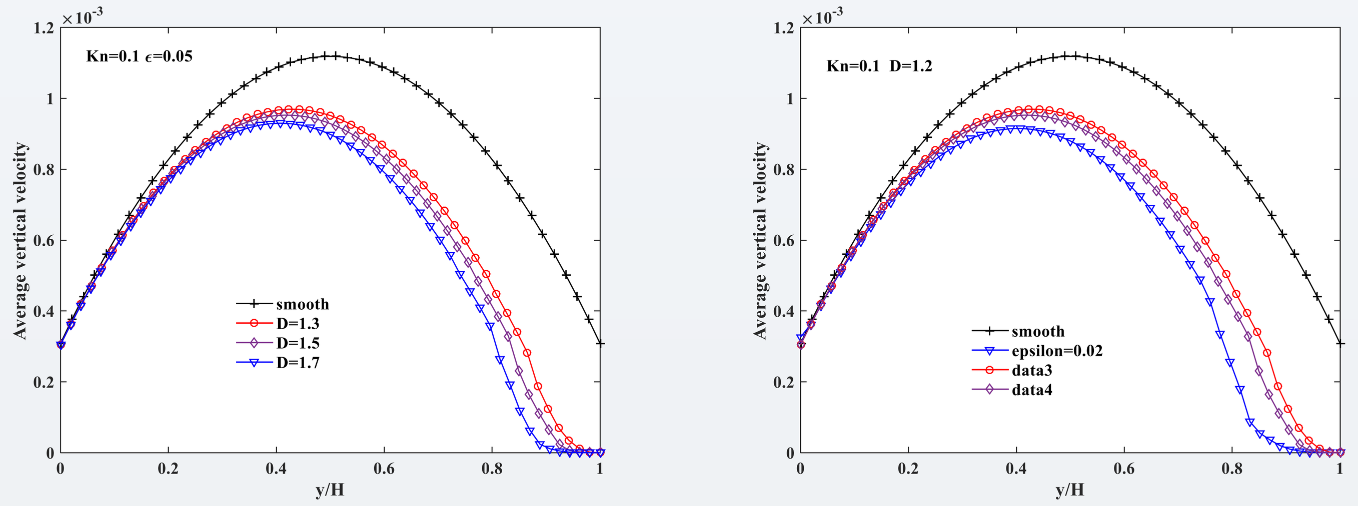
ε=7%

- The deviation of the velocity profile in a rough microchannel from that in a smooth microchannel is increasingly evident as the Knudsen number increases. When it comes to a large Knudsen number, large discrepancies of gas velocity profiles are observed between the smooth and rough microchannel. The role of surface-gas collisions in gas flow as compared with intermolecular collisions is being enhanced with increasing Knudsen number.
- Irrespective of gas flow regime, the gas velocities in the vicinity of rough surfaces are all close to zero, which is opposed to smooth microchannel where the slip velocity increases for a larger Knudsen number.
- The cavities in rough surfaces restrict the motion ability of gas close to the wall, hence resulting in the reduction of boundary velocity slip, which in turn decreases the bulk flow velocity.



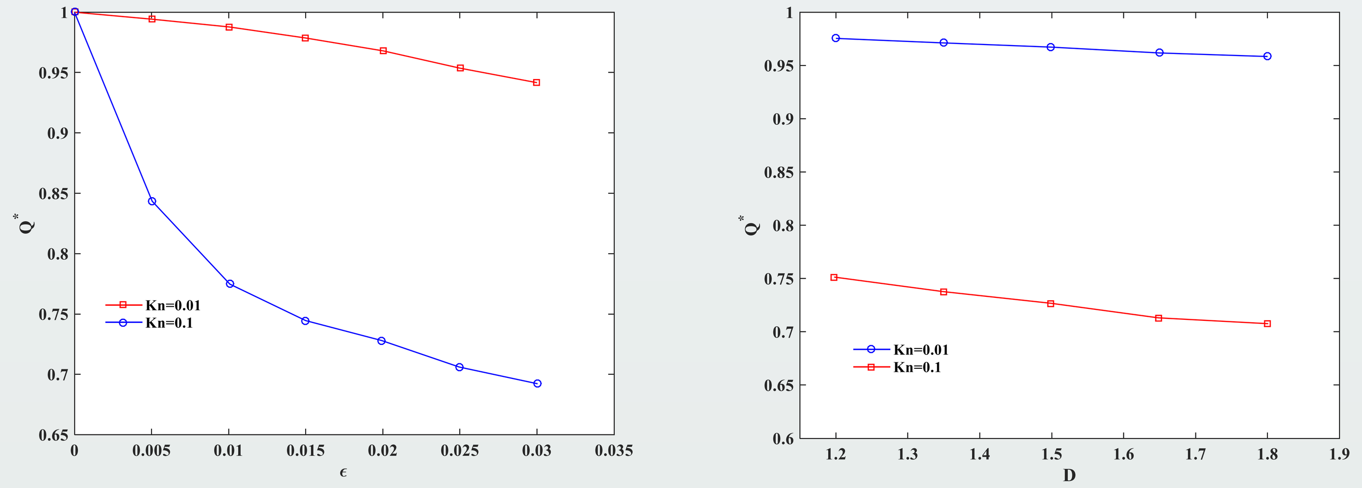
- The velocity profiles varies with the roughness height, and this variation tends to be evident at large Kn. However, for rough surfaces with different fractal dimensions, the velocity profiles are close to each other even at large Kn.
- Comparing to the roughness height, the effect of fractal dimension on the velocity profiles is less significant. The variation of surface irregularity shows a tiny effect on bulk gas flow in microchannel.





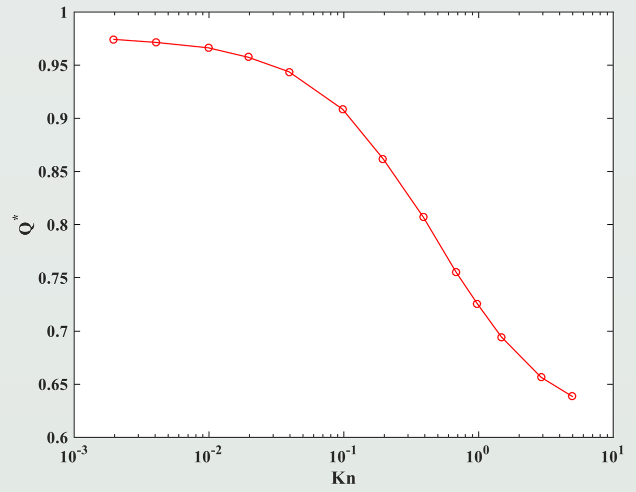
b) Effect of rough surface

- The self-affine fractal dimension and statistical roughness height are two crucial factors for the roughness of the wall, which directly determine the surface topography.
- The mass flow rate decreases monotonously with increasing roughness height. Gas flow behavior in the transition flow regime is more sensitive to roughness height than that in the slip flow regime.
- For increased rarefaction, the surface-gas interaction is increasingly significant for gas flow in a microchannel while the gas molecular interaction is reduced. The surface-gas interaction starts to dominate the gas flow behavior, when the Knudsen layer is o the same order of magnitude as a mean free path.



c) Effect of rarefaction

- There is a trend toward the decrease in the relative mass flow rate Q* of rarefied gas flow as Knudsen number increases. Increases in Knudsen number lead to a large portion of the flow passage being occupied by the Knudsen layer.
- The surface roughness effect becomes more significant in microscale gas flow with enhanced rarefaction. In particular, the surface roughness is of considerable importance to the gas flow in the transition flow regime owing to the dominance of the surface-gas interaction in the Knudsen layer.



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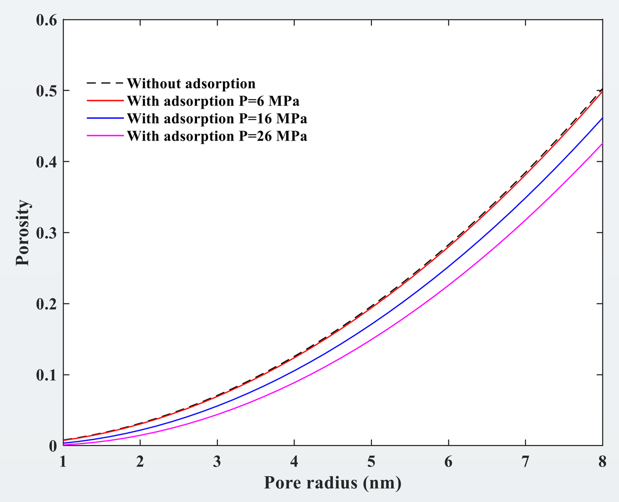
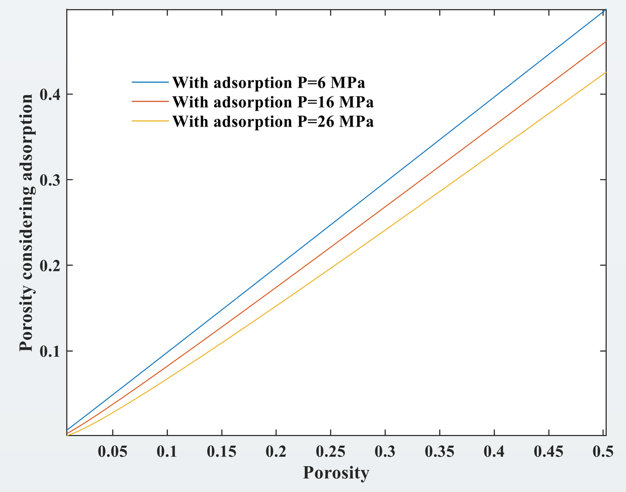
3. Adsorption effect and upscaling method

d) Pressure-dependent thickness of adsorption layer

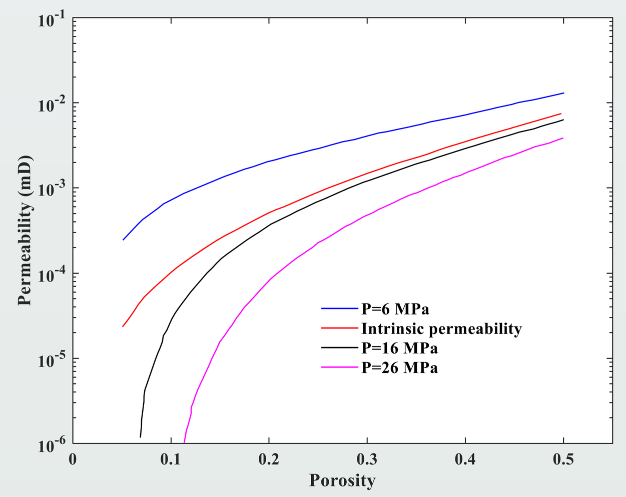
The thickness of the adsorption layer is a function of the pressure.

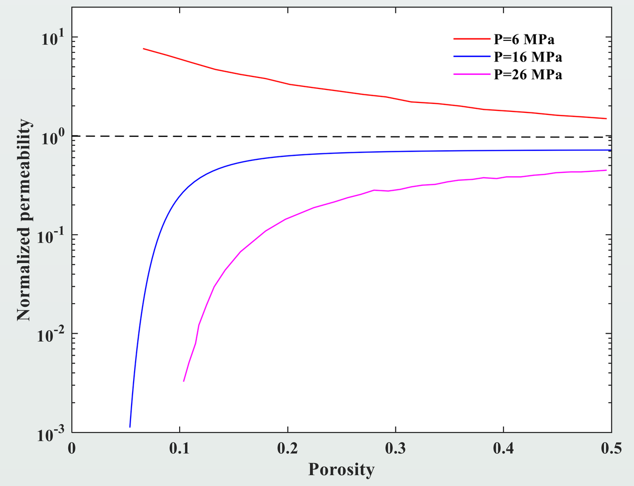
$$\delta = \frac{P - P_1}{P_1 - P_0}(\delta_1 - \delta_0)$$





- The existence of adsorption will reduce the actual pore size and the higher the pressure, the lower the actual pore size.
- The intrinsic permeability is the permeability of liquid through the porous medium, in which slip is absent, and thus is not affected by the pressure. The intrinsic permeability and the apparent permeability decrease as the porosity decrease.
- The apparent permeability is higher than the intrinsic permeability, under a lower pressure. However, under a higher pressure, the apparent permeability is lower than the intrinsic permeability.
- Slippage and adsorption have opposite effects on gas flow, with the former one enhancing the gas flow while the latter one reducing the pore size and thus weakening the gas flow.





- The variation of normalized apparent permeability, however, presents different trends under different pressures. Under a low pressure, the normalized apparent permeability increases as the porosity decreases, wile the trend is reverse for a high pressure.
- At a low pressure, the adsorbed layer has neglected effect on gas flow and the slippage dominates. As porosity decreases, the pore size decreases, thus normalized apparent permeability increases. As the pressure increases, the adsorbed layer becomes increasingly thicker. The pore even will be completely filled by the adsorbed layer. Therefore, the normalized apparent permeability decreases as the porosity decreases under high pressure.

3) Upscaling

a) Upscaling method

The pore-scale properties, including the microstructure geometry effect, will propagate to the field scale through iterations. It can be interpreted that there is a hydraulic fracture at right boundary which has good connection to the wellbore, so its pressure equals the bottom hole pressure.

① Uniformly divide the porous media into several zones. In the center of each zone, take a REV bounded within the black square.

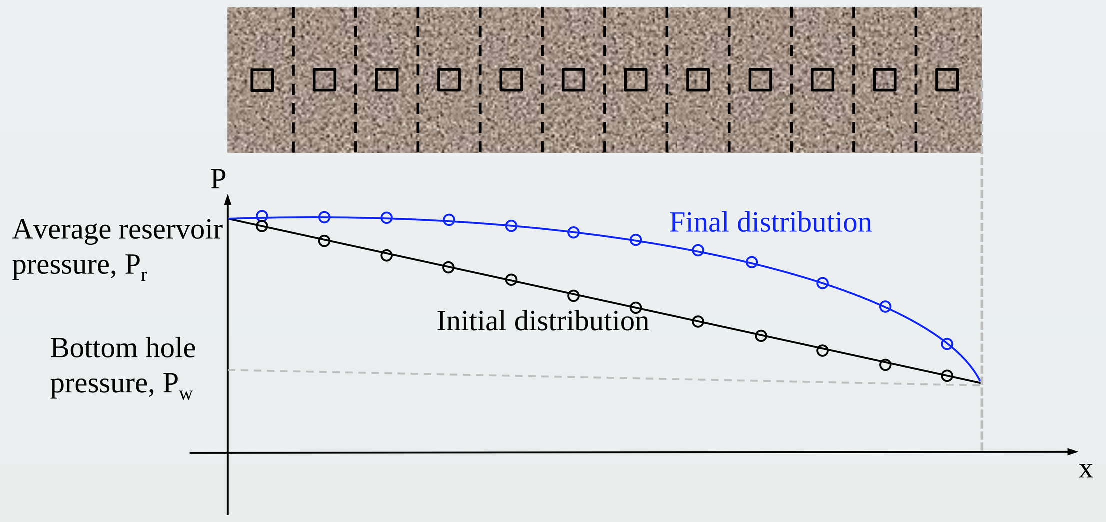
② Given an initial pressure distribution along the porous media.

③ Determine the center pressure and pressure difference between the inlet and outlet of each REV.

④ Simulate the flow in each REV under the given pressure difference and obtain the mass flow rate.

⑤ Update the pressure distribution based on the mass flow rate.

⑥ Repeat ③~⑤ until the pressure distribution is converged. Then output the results.



b) Updating method

For steady state flow without internal fluid source or sink, the target variable is the mass flow rate restricted from the mass balance law. For the ith REV, an effective updating method is:

$$\Delta P_i^{new} = \Delta P_i - \frac{1}{N_{REV}}(P_r - P_w)(q_i - g_i)/\bar{q}$$

$$P_i^{new} = P - \sum_{j=1}^{i}\Delta P_j^{new} + \frac{1}{2}\Delta P_i^{new}$$

where g_i is a new parameter determined by

$$g_1 = \frac{1}{2}C\left.\frac{d\rho}{dP}\right|_{P=P_r}$$

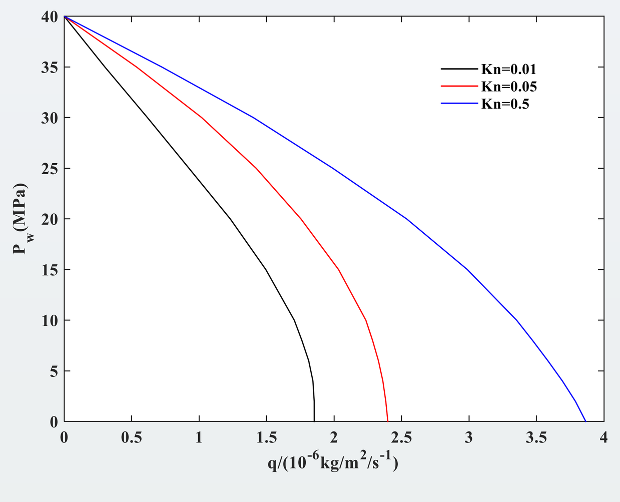
$$g_{i+1} - g_i = C\left.\frac{d\rho}{dP}\right|_{P=P_i}$$

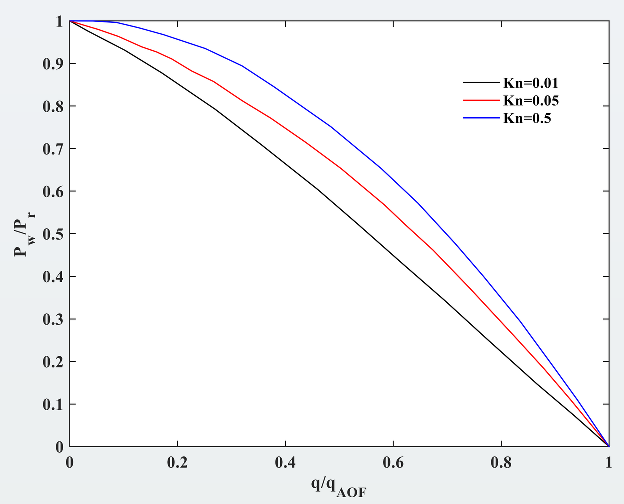
$$\sum_i g_i = \sum_i q_i$$

c) Inflow performance relationship

The inflow performance relationship describes the relation between the gas production and the bottom hold pressure P_w, under a constant average reservoir pressure P_r, IPR is of vital significance in analyzing the gas storage, predicting the gas production and optimizing the well arrangement.

$$q = q_{AOF}\left(1 - \frac{P_w^2}{P_r^2}\right)$$



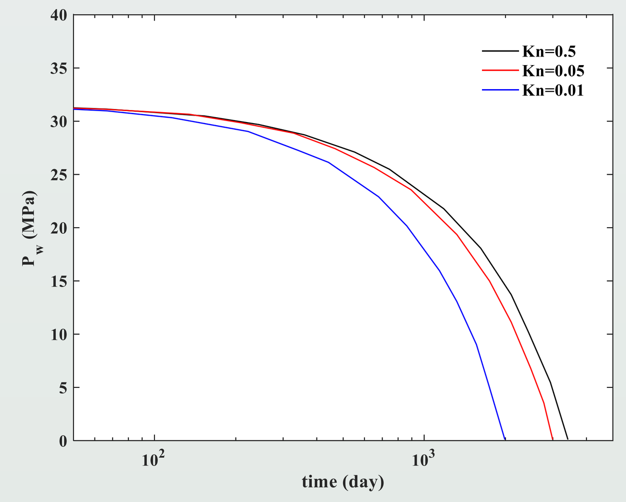


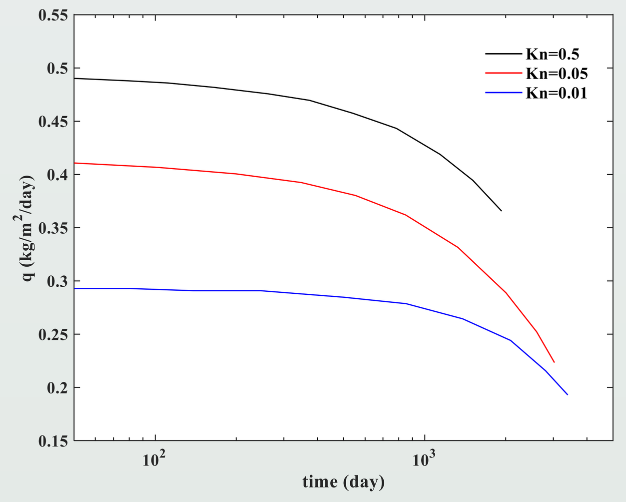
d) Decline curve analysis

Decline curve analysis is a widely concerned issue in natural gas engineering. Through a spline interpolation, the functions $dp/dt(P_w)$ and q_w are determined from the discrete simulation results. Thus the time is inversely integrated as:

$$t(P_w) = \int_{P_w^{initial}}^{P_w}\frac{1}{\frac{dP}{dt}(P_w)}dP_w$$

It is seen that the gas production will be overestimated at the early stage and underestimated at the late stage when neglecting the rarefaction effect and compressibility effect. At the early stage, the compressibility effect is dominant since the gas pressure is high, which results in larger gas viscosity and thus lower gas production. In contrast, the pressure becomes low at the late stage, leading to the dominance of rarefaction effect, which makes the gas production higher.





Conclusion

- Permeability of the IOM increases with the increase of pore radius and the decrease of pressure. Permeability of the OM shows a similar trend with pressure and pore radius to that of the IOM
- Surface diffusion in the OM can have a more important role than Knudsen diffusion and convection flow in determining the apparent permeability at low pressure.
- Permeability shows strong dependence on the value of Langmuir parameters and surface diffusivity.
- The surface roughness effect on gas flow behaviors becomes more significant in rarefied gas flow with the increase of Knudsen number.
- Increases in Knudsen number lead to a large portion of the flow passage occupied by the Knudsen layer and hence cause the surface-gas interaction to be more important for gas flow confined in micro-space.
- The gas flow behavior in the transition flow regime is more sensitive to roughness height than that in the slip flow regime. In addition, the influence of fractal dimension on rarefied gas flow behavior is less significant than roughness height.
- The velocity profile in a rough microchannel that deviates from smooth microchannel is increasingly evident as the Knudsen number increases. The gas velocities in the vicinity of rough surfaces are all close to zero, which is opposed to smooth microchannel where the slip velocity increases for a larger Knudsen number.
- Adsorption layer reduce the actual porosity of the nanometer tube. The permeability, considering the overall effects of adsorption and slippage, shows different tendencies under different pressures. Under a low pressure , the normalized permeability increases as the porosity decreases and the value is all above unity. While the trend is reverse for a high pressure.
- In the study of inflow performance relationship, it is uncovered that high Knudsen number leads to a larger mass flow rate under the same pressure condition. When Knudsen number is 0.5, the absolute open flow rate is $3.9*10^{-6}$kg/m²/s, which is 2.67 times larger than non-slip model. In decline curve analysis, micro-scale effect becomes dominant at late stage, which results in an underestimation of gas production. This is because at the late stage the pressure becomes very low, leading to a high Knudsen number, which makes the gas production higher.

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