Multiscale Lattice Boltzmann Simulation of the Kinetics Process of Methane Desorption-Diffusion in Coal

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1. INTRODUCTION

Coalbed methane (CBM) is an essential and promising energy resource that is considered as a substitute for oil and has attracted great interest from both the research community and commercial sector all over the world in recent years.1 Unlike conventional natural gas (CNG), CBM is generated from the coal seam and stored by physisorption in the nanopores of coal. Therefore, coal is both the resource and reservoir of CBM, and the premise of CBM exploitation is to desorb methane from coal, which makes it difficult for CBM production.2 Nowadays, it is essential to understand the mechanism of methane storage and migration in coal.

Coal is a tight porous medium with a huge surface area and complicated pore structure, which has a strong adsorption capacity for methane.3,4 The highly heterogeneous structural properties of coal vary depending on the burial depth, hydrogeological environment, and formation process, resulting in its pore sizes varying from a couple of nanometers to more than 1 μm. Generally, coal is considered as a double pore system consisting of primary and secondary pore systems, where the primary pore system mainly refers to the nanopore-rich coal matrix, while the secondary pore system refers to the macropore or microfracture zone.5

The mechanism of gas migration in pore systems is closely related to pore size. Pores of porous media can be categorized as micropores (less than 2 nm), mesopores (2−50 nm), and macropores (more than 50 nm) according to pore size.6 Previous research7 has shown that coal contains a larger amount of micropores and a smaller number of macropores. The large specific surface area of micropores and mesopores can provide a massive storage space for adsorbed gas molecules. However, the specific surface area contributed by macropores is very small compared to micropores and mesopores, and the adsorption ability is generally disregarded, offering just as a channel to enable the migration of methane particles between the bulk phase and the interior of the coal grain. Meng et al.7 investigated the distribution of pore size of coal samples from the Xishan coal mining block (in China) via
utilizing the static nitrogen adsorption capacity technique (SY/T6154-1995). The outcomes suggested that the mean radii of pores of the coal samples varied from 7.729 to 15.338 nm and the biggest percentage was that of micropores accounting for 65.4%. Zhao et al.26 analyzed six sets of middle- and high-rank coal samples by the employment of the synchrotron small-angle X-ray scattering (SAXS) technique and discovered that the mean sizes of pores ranged from 2.9 to 23.1 nm.

Methane flow in coal reservoirs typically includes a variety of physical activities, consisting of fluid dynamics, thermodynamics, and chemical kinetics, along with electrodynamics because the majority of surfaces of natural media are charged. All of these processes are eventually controlled by the interface phenomena of pore-scale. It is challenging to characterize the structure of the pore because of the wide distribution of pore size of the coal matrix, which makes it extra difficult to comprehend the mechanism of methane migration in coal. The length range of the coal matrix is much higher than the sizes of regular pore or mineral particles, and the size of the pore inside the matrix is fairly diverse from that of outside. The feature of the typical dual-porosity of the coal seam makes the storage and migration of coalbed methane very complex, and accurately characterizing the methane migration mechanism is a crucial question in coalbed methane production.3,10 Consequently, the continuity formulas founded on the theory of spatial average are generally utilized to characterize the structure of the coal matrix, while its spatial heterogeneity in smaller ranges is disregarded.11 Presently, the most usual strategy to simplify the structure of coal is to consider the matrix as a bidisperse porous medium with ununiform geometry and a homogeneous material.12–17 The homogeneous portion stands for the coal matrix and usually does not consider certain structural and distribution features of its inner micropores, just its statistical features, i.e., porosity and average pore size.

Generally, methane migration in coal is regarded to take place at two levels: (1) gas flow via macropore or fracture systems and (2) the diffusion, adsorption, and desorption of gas in the matrix. In a macroscopic approach, the gas flow through the fracture system is pressure-driven and can be explained by the Navier–Stokes formula, while the gas diffusion in the matrix is presumed to be concentration-driven. Depending on the Knudsen number (the ratio of the average free path of gas particles to the average pore radius of porous media), the gas transport mechanisms can be categorized as bulk diffusion, Knudsen diffusion, and surface diffusion.18,19 For Fick diffusion, the collision between gas molecules is dominant, while in Knudsen diffusion, the collision between gas molecules and the pore wall surface of the matrix is dominant. According to the Knudsen number of coal, the transfer of methane molecules in macropores/fractures of coal can be defined by Fick’s law, while those in the micro- or mesopores of the coal matrix are mainly Knudsen diffusion and surface diffusion, respectively.20,21

The adsorption-desorption behavior of gases is one of the primary reasons why CBM differs from CNG, and it involves some complex mechanisms. In general, there are van der Waals forces and chemical bonding forces between gases and solid. Chemisorption is an irreversible chemical reaction that integrates gas molecules with solid particles through chemical bonding to form a new molecular structure. The adsorption of methane on coal is essentially a reversible physical reaction that combines solid particles on the internal surface of coal matrix pores with methane molecules via van der Waals forces.22–25 The inner surface of the pores of the coal matrix has a large number of adsorption sites, which contribute dramatically to the storage of methane. Previous research suggested that the quantity of gas in the adsorbed state represents greater than 85% of the total gas quantity.26 For a normal CBM extraction procedure, free gas in the fractures or macropores of the coal seam diffuses out initially after water drainage and a fast gas production phase takes place.27 Nevertheless, as a result of the restriction of the diffusivity and the desorption kinetics of methane molecules on the inner surface of the micropore, methane desorption will certainly control the succeeding procedure of gas production.28,29 A lot of previous studies on the adsorption and desorption characteristics of gases in coal are mainly based on isothermal adsorption equations, including the Langmuir isothermal adsorption equation, which can provide essential recommendations for gas production assessment and mathematical modeling. Nevertheless, the obtained isothermal information can just supply macroscopic and static information and disregard the dynamic procedure during gas adsorption and desorption.30–32 Do and Wang33 measured adsorption and desorption equilibrium data on activated carbon and discovered the existence of the adsorption delay phenomenon. The outcomes of their research showed that adsorption on the pore surface of activated carbon is heterogeneous, which causes the truth that the adsorption of gases does not take place instantly and it takes some time to get to adsorption-desorption equilibrium, in which case the time consumption of gas adsorption and desorption is close to gas diffusion.

The present work developed a lattice Boltzmann method (LBM) with a dual distribution formula to deal with the coupled Navier–Stokes formula and advection–diffusion formula. In the simulation, we concentrated on the modeling of methane migration in the multiscale porous media of coal, which also considered the gas viscous flow and Fick diffusion in fractures/macropores and the gas Knudsen diffusion in micropores/mesopores of the coal matrix, and the adsorption–desorption kinetics of methane-coal.

2. MULTISCALE LB MODEL FOR GAS DIFFUSION-ADSORPTION-DESORPTION IN POROUS MEDIA

2.1. The Macroscopic Governing Equation for Fluid Flow and the Gas Diffusion-Reaction. The Navier–Stokes equation is based on the assumption of a continuous medium, which reflects the basic physical law of macroscopic fluid flow.34 The Navier–Stokes equation with the condition of isothermal and incompressibility can be expressed as

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0
\] (1)

\[
\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot [\mu \nabla \mathbf{u} + \nabla \mathbf{u}^T]
\] (2)

where \( \rho \) is the fluid density, \( \mathbf{u} \) is velocity, \( t \) is time, \( p \) is the pressure, and \( \mu \) is the kinematic viscosity coefficient.

On the macroscale, if the concentration of solute is small enough while the impact on the density and velocity of solution can be ignored, the process of mass transfer with the reaction can be described by the advection–diffusion formula:35,36

\[
\frac{\partial (\rho \mathbf{u} \cdot \mathbf{c})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \cdot \mathbf{c} \mathbf{u}) = \nabla \cdot (D \nabla \mathbf{c}) + \mathbf{S}
\] (3)

where \( \rho \mathbf{u} \cdot \mathbf{c} \mathbf{u} \) is the advective flux, \( D \) is the diffusivity matrix, and \( \mathbf{S} \) is the source term.
\[
\frac{\partial C}{\partial t} + \nabla \cdot (C \cdot \mathbf{u}) = \nabla \cdot (D \nabla C) + R,
\]

where \( C \) is the concentration of the solute, \( D \) is the diffusion coefficient, and \( R \) is the source/sink term associated with gas adsorption/desorption.

### 2.2. The LB Equation for Fluid Flow

The lattice Boltzmann method is founded on the mesoscopic kinetic model that has the characteristics of the microscopic approach with fewer assumptions and the advantage of the macroscopic approach without caring about the details of molecular motion and has greater advantages and potential in handling complex flow issues with multiscale and multiphysics.

Because the gas velocity under regular reservoir conditions is small enough while the Mach number is much lower than 0.3, methane flow in coal can be supposed under the incompressible limit. Therefore, the LB method for gas viscous flow in tight coal seams can be denoted as follows:

\[
f_i(x + \mathbf{e}_i \cdot \Delta t + \delta_i) - f_i(x, t) = -\frac{1}{\tau} [f_i(x, t) - f_i^{eq}(x, t)]
\]

with

\[
f_i^{eq} = \rho \omega_c \left[ 1 + \frac{\mathbf{e}_i \cdot \mathbf{u}}{c_s^2} + \frac{\mathbf{u} \cdot \mathbf{u}}{2c_s^4} \right]
\]

where \( f_i \) is the discrete density distribution function, \( f_i^{eq} \) is the local equilibrium function, \( \omega_c \) is the discrete velocity of the particle, \( c_s \) is the lattice sound velocity, \( \tau \) is the relaxation time, \( \omega \) is the weight coefficient, and \( \delta_i \) is the time step.

### 2.3. The LB Equation for the Gas Diffusion-Reaction

The passive scalar LB equation is utilized to describe the diffusion of gas in the coal reservoir with adsorption and desorption:

\[
g_i(x + \mathbf{e}_i \cdot \Delta t + \delta_i) - g_i(x, t) = -\frac{1}{\tau^*} [g_i(x, t) - g_i^{eq}(x, t)] + \omega R_i \delta_i
\]

where \( g_i \) is a discrete concentration distribution function, \( g_i^{eq} \) is the corresponding local equilibrium distribution function, and \( \tau^* \) is the diffusion-related relaxation time.

Since the lattice Boltzmann equation is a theory that explains the regulations of fluid movement, it should follow the Navier–Stokes formula under certain conditions. In the standard LBM, the gas density and velocity on the macroscopic approach can be denoted as \( \rho = \sum f_i \rho \) and \( \mathbf{u} = \sum f_i \mathbf{e}_i \mathbf{u} \), respectively. With the conditions of \( p = c_s^2 \rho \) and \( \mu = c_s^4 (\tau - 0.5) \delta_i \) and the employment of the Chapman–Enskog method, eqs 4 and 5 can recover the Navier–Stokes formulas, i.e., eqs 1 and 2 under the incompressible limit. Similarly, the concentration can be defined as \( C = \sum g_i \) and using the LB equation of the gas diffusion-reaction with the condition of \( D_i = c_s^2 (\tau - 0.5) \delta_i \) eqs 6 and 7 can recover the advection–diffusion formula, i.e., eq 3 with a source/sink term.

For methane migration in a multiscale system related to the tight coal, the diffusion coefficients include the Fick diffusion coefficient (FDC) and Knudsen diffusion coefficient (KDC). It should be mentioned that the surface diffusion of methane is neglected due to the fact that the diffusional activated energy is insufficient in the gas desorption process. In practice, the FDC can be acquired through measurement and the KDC can be obtained following the model of the parallel capillary tube of porous media:

\[
D_k = \frac{2r}{3} \sqrt{\frac{8RT}{\pi M}}
\]

where \( R \) is the gas constant, \( r \) is the average radius of the capillary tube, \( M \) is the molar mass of the methane, and \( T \) is the temperature.

The impacts of porosity, as well as tortuosity of the porous media, also need to be taken into consideration as a result of the complicated geometric structure of coal. Consequently, the effective KDC can be given by

\[
D_{lp} = \frac{\epsilon_{m,0}}{\tau_w} D_k
\]

where \( \tau_w \) is the tortuosity and \( \epsilon_{m,0} \) is the original matrix porosity.

### 2.4. Langmuir Kinetic Formula of Gas Adsorption and Desorption

At present, the Langmuir isothermal adsorption model is the most commonly used one and has been applied to the methane-coal adsorption. In this paper, we employed the Langmuir kinetic formula governing the dynamic process of gas adsorption and desorption:

\[
\frac{\partial V}{\partial t} = k_a C (V_L - V) - k_d V
\]

where \( V \) is the adsorbed amount, \( C \) is the gas concentration, \( V_L \) is the Langmuir volume, and \( k_a \) and \( k_d \) are the adsorption and desorption rate constants, respectively.

The adsorption and desorption between methane and coal are typically reversible physisorption. At a certain moment, when \( \frac{\partial V}{\partial t} < 0 \), the gas desorption from pores because of the adsorption rate is less than the desorption rate; similarly, if \( \frac{\partial V}{\partial t} > 0 \), the quantity of net gas adsorbed rises; when \( \frac{\partial V}{\partial t} = 0 \), adsorption and desorption reach equilibrium, and eq 10 can be rewritten to the Langmuir isotherm adsorption formula,

\[
V = \frac{V_L P}{p + P_L} = \frac{V_L C}{C + C_L}
\]

where \( P \) is the gas pressure, \( p = CM_c^2 \), \( P_L \) is the Langmuir pressure, and \( C_L \) is the concentration corresponding to the Langmuir pressure, \( C_L = k_d / k_a \).

It should be noted that \( P_L \) is in proportion to the ratio of \( k_a \) to \( k_d \) and independent of the quantity of both. The values of \( K_d \) and \( P_L \) can be obtained from the experiment, and one can be acquired from the other two of them.

To realize the adaptive transformation of gas adsorption and desorption in each adsorption site, a source/sink term founded on He and Li’s model was introduced. Then, the Langmuir kinetics formula can be combined into the LB model via the source/sink term,

\[
R_s = \frac{\partial V}{\partial t} = k_a C (V_L - V) - k_d V
\]

The adsorbed and desorbed quantity of gas is renewed with time steps, and with the application of a first-order difference scheme of eq 10, the new quantity can be acquired,

\[
V_{t+1} = V + \delta_t [k_a C (V_L - V) - k_d V]
\]
The bidispersed porous media that characterize the structure of the coal are composed of clusters of tiny coal particles, as displayed in Figure 1. In the framework, there are numerous micro- and macropores within and between the clusters of particles, respectively. The verification of the LB model can be seen in Appendix A.

3. RESULTS AND DISCUSSION

3.1. The Effect of the Geometric Properties of the Coal Matrix on the Gas Desorption-Diffusion Process.

To study the impact of geometric characteristics of the coal matrix on the methane desorption-diffusion process, five groups of bidispersed porous media were constructed; their specific surface areas and porosities are shown in Figure 2.

![Figure 2. Simplified 2D reconstructed geometry of the coal matrix: (a) G-1 (S = 0.4, \(\varepsilon_f = 0.64\)), (b) G-2 (S = 0.27, \(\varepsilon_f = 0.64\)), (c) G-3 (S = 0.13, \(\varepsilon_f = 0.64\)), (d) G-4 (S = 0.13, \(\varepsilon_f = 0.55\)), and (e) G-5 (S = 0.13, \(\varepsilon_f = 0.44\)). The matrix porosity of the solid matrix is 0.05.](image-url)

Figure 3 shows the magnitude distribution of (a) gas concentration and (b) the adsorbed amount after desorbing at 500,000 steps. In Figure 3a, a stable concentration gradient distribution has been formed in the field. Compared with G1–G3, the concentration distribution of G1 is more uniform; however, G2 presents an uneven “waveform” near the dislocation matrix and the phenomenon in G3 is more obvious. The corresponding concentration distribution of G3–G5 is slightly different, but the difference is not distinct. In Figure 3b, due to the concentration distribution being stable, the rapid desorption of gas is near the end and the distribution of the residual adsorbed amount is similar to the concentration, showing a stable gradient distribution. The difference between G1 and G3 is obvious, and gas desorption in G1 is more uniform, while the closer the gas is to the low concentration outlet, the gas in the matrix of G3 desorbs faster and an “arc shape” desorption-diffusion path is formed.

Figure 4 shows the magnitude of the total adsorbed amount of G1–G5 at 500,000 steps. Due to the same \(\varepsilon_f\) of G1–G3, namely, the total volume of the matrix is identical, the initial total adsorbed amounts of G1–G3 are equal. However, with a larger S, the gas desorption is faster. This is because the larger of the exceptionally poor permeability and small porosity, the flow velocity of methane within the coal grain clusters is low enough to consider the clusters as impermeable (\(u = 0\)). The detailed typical parameters of coal and methane in the simulation are displayed in Table 1. The simulation outcomes are demonstrated in Figure 3.

![Figure 1. Diagram of the bidispersed porous media characterizing the coal structure.](image-url)

![Figure 3.](image-url)

![Figure 4.](image-url)

### Table 1. Typical Parameters of Coal and Methane in the Simulation

| Parameter                  | Value                |
|----------------------------|----------------------|
| Simulation area L × L      | 2 × 2                |
| Average pore radius of the coal matrix (m) | 2 × 10⁻⁹ |
| Methane density \(\rho_m\) (kg/m³) | 43.6               |
| Methane viscosity \(\mu\) (Pa·s) | 1.26 × 10⁻⁵        |
| Coal density \(\rho_c\) (kg/m³) | 1400               |
| Fick coefficient \(D_f\) (m²/s) | 2.0 × 10⁻⁸        |
| Langmuir pressure \(P_l\) (Pa) | 2 × 10⁶           |
| Langmuir volume \(V_l\) (m³/m³) | 42                 |
| Desorption rate constant of methane \(k_d\) (/s) | 2.94 × 10⁸      |
| Pressure gradient \(\nabla p\) (MPa/m) | 0.1             |

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the S, the higher fragmentation of the matrix (the matrix with a smaller volume) is; the gas desorption-diffusion path will be shorter. If the desorption time is long enough, the residual total adsorption amount of G1−G3 will eventually be the same.

In addition, G3−G5 with the same S indicate that the volume of each matrix block is consistent. With the increase of εf, the total volume of the matrix in the system decreases. As can be seen from Figure 4, when the εf increases, the initial total adsorbed amount decreases, but the rates of gas desorption of the three are identical, which results in the difference between G1, G2, and G3 that cannot be observed in Figure 3.

In the exploitation of coalbed methane, the employment of hydraulic fracturing technology to increase production has been widely concerned. By hydraulic fracturing, the fractures of the coal reservoir will have a second development, which can effectively improve the specific surface area of coal and may make the pore connection better and the gas desorption-diffusion efficient. In addition, hydraulic fracturing will not reduce the matrix area; therefore, the initial adsorbed amount will not decrease.

### 3.2. The Effect of Gas Flow and Diffusion of Macropores/Fractures on the Gas Desorption-Diffusion Process

The success of coalbed methane exploitation relies on the migration performance of methane in coal seams, which relates to gas flow and diffusion. Methane diffusivity varies greatly in different coal seams, temperatures, pressure, etc. Methane flow is associated with the pressure gradient of the coal reservoir, which depends on the water drainage strength of the wellbore. Because of the dual-porosity structure of the coal reservoir, we only consider the impact of gas flow and diffusion of macropores/fractures on the gas desorption-diffusion process in this section, and additional issues are identical with Section 3.1. The simulation outcomes can be observed from Figures 5 and 6.

Figure 5 shows the combined effect of gas flow and diffusion on the desorption-diffusion process. It can be found that when gas diffusivity is 0.01D0, the gas desorption rate varies greatly under different flow velocities, which increases with the increase of flow velocity. However, the trend is not obvious when the fluid velocity reaches 10u0. As to gas diffusivity up to D0, the desorption process is mostly consistent under the different magnitudes of the flow velocity. On this condition, the effect of fluid velocity on desorption-diffusion can be ignored.

Figure 6 shows the influence of the FDC on the desorption-diffusion process. As the FDC increases, gas transport is more efficient and the gas concentration around the matrix updates faster, which will accelerate the rate of gas desorption. However, when the FDC increases to a certain extent (e.g., 10D0), due to the limitations of gas diffusivity and desorption rate in the matrix, the enhancement of the FDC on the gas desorption process becomes smaller. Also, when the FDC is...
less than $100D_s$, the effect of gas diffusivity of macropores/fractures on the desorption-diffusion process can be neglected.

The above results indicated that the flow and diffusion of methane are closely related to each other in the desorption-diffusion process. When the gas diffusivity is poor, the gas desorption can be effectively accelerated by increasing the drainage intensity, but when the gas diffusivity is good, increasing the flow velocity has little effect on the gas desorption. In productivity prediction or experiment, if the estimated gas diffusion coefficient is less than the order of $10^{-5}$ m$^2$/s, more attention should be paid to its accuracy; otherwise, the obtained results may have a large deviation from the real value.

3.3. The Effect of Gas Diffusion and Adsorption-Desorption in the Coal Matrix on the Gas Desorption-Diffusion Process. As a kind of tight porous medium, the gas diffusivity inside the coal matrix is related to porosity, pore diameter, tortuosity, and pore distribution; however, these parameters are usually difficult to measure. Researchers generally use the average pore diameter to describe the performance of gas transport in porous media. In the simulation, we assume that the gas transport inside the coal matrix is Knudsen diffusion, and the effect of the KDC on the gas desorption-diffusion process was investigated by varying the average pore size, and the impacts of the key parameters that control gas adsorption-desorption on the gas desorption-diffusion process are also studied. The input parameters in the simulation can be seen in Table 1, and the results are shown in Figures 7–9.

Figure 7 shows the variety of total adsorbed amounts when the average pore size of the coal matrix is different. As can be seen, with a larger $r$, gas desorption is faster, owing to the fact that the KDC increases with $r$, making the gas concentration near the adsorption sites update more efficiently. However, the decay rate of the gas adsorbed amount will slow down with increasing $r$, which is similar to the trend of the FDC. Langmuir pressure and volume are two key parameters in the Langmuir isothermal adsorption formula. To investigate the impact of Langmuir pressure and volume on the process of methane desorption-diffusion, we utilized four groups of typical Langmuir pressure and volume data of coal reservoirs and acquired the results as displayed in Figure 8. It ought to be mentioned that our model is founded on the Langmuir adsorption kinetic formula and the Langmuir pressure is not included, but it can be quickly calculated from the adsorption rate constant and desorption rate constant.

The Langmuir volume of low-rank coal is usually less than those of medium- and high-rank coals. A previous study\textsuperscript{23} indicates that the methane adsorption ability of low-rank coal is generally dominated by functional groups, while that of high-

Figure 6. Effect of the FDC on the desorption-diffusion process.
rank coal is primarily controlled by the construction of micropores and aromatic nucleus. With the rise of coal rank, the aromatic structure in coal condenses into the macromolecular structure, which makes the adsorption ability improve. Furthermore, the pore size distribution of high-rank coal varied dramatically and the variety of micropores enhanced. Medium- and high-rank coals are abundant in micropores and have a high specific surface area, which can supply a lot of adsorption sites for methane, bringing about a bigger Langmuir volume.

It can be observed from Figure 8a that the larger the $V_L$, the larger the initial total adsorbed amount, which is consistent with the previous study. However, the decay of the total adsorbed amount is not affected due to the fact that the gas adsorption and desorption rates remain unchanged with different $V_L$ values.

In a similar condition, we obtained the total adsorbed amount under different Langmuir pressures as can be observed in Figure 8b. Contrary to the effect of $V_L$, with a larger $P_L$, the total adsorbed amount will be smaller, which is consistent with the result predicted by the Langmuir isothermal adsorption equation. Similarly, with a Langmuir pressure matching the original adsorbed quantity, the variation of $P_L$ has no impact on the adsorption and desorption rates.

However, $P_L$ is related to the proportion of the desorption rate constant to the adsorption rate constant, which mirrors the difficulty of methane desorption in coal, and a bigger Langmuir pressure implies that the adsorbed gas is easier to desorb from the internal surface of nanopores in the coal matrix, which follows the results displayed in Figure 8c.

To study the influence of the magnitude of adsorption and desorption rates on the process of methane desorption-diffusion, we employed four groups of adsorption and desorption rate constants that cover a wide extent in the simulation and obtained the results as shown in Figure 9.

Since $P_L (k_d/k_a)$ remains unchanged, the equilibrium state between the adsorption and desorption of gas is fixed, and the variation of adsorption and desorption rate constants will only change the update rate of gas adsorption and desorption in dynamic equilibrium at the adsorption site. It can be found that the adsorption/desorption rate constant has a significant effect on the desorption-diffusion process. When the adsorption/desorption rate constant is very small ($0.01k_d$),
the gas desorption is quite slow. With the increase of the constant, its effect on the desorption-diffusion process becomes smaller. As it reaches $10k_d$, the desorption-diffusion process is basically no longer limited by the desorption rate.

In the typical range of average pore size of coal,7,8 the gas desorption rate increases with the growth of pore size, and a wider influencing range of fracturing can significantly broaden the average pore size. In addition, the low-rank coal with bigger average pore size has more advantages in the activity of methane desorption-diffusion. Along with the rise of coal rank, the Langmuir volume boosts, but the Langmuir pressure initially drops and after that, enhances. Consequently, because the high-rank coal has a larger adsorption capacity and with the reduction of reservoir pressure, the low- and high-rank coals more easily desorb methane than medium-rank coal. In the kinetic study of the coalbed methane desorption-diffusion process, the accuracy of the obtained results may depend on the adsorption/desorption rate constant if the desorption rate constant is less than $10^7$ 1/s.

In the investigation, several crucial parameters of coal and methane, such as gas diffusion coefficient, Langmuir volume and pressure, and desorption rate constants, have a reasonably wide range coverage. Furthermore, because lots of features, including constituting components, geological environment, development of fractures, etc., of coal are ignored in the multiscale simulation, the outcomes acquired can be extensively utilized in the mining of coalbed methane.

4. CONCLUSIONS

In the paper, we concentrated on the modeling of methane migration in the multiscale porous media of coal, which also considered the gas viscous flow and Fick diffusion in fractures/macropores and the gas Knudsen diffusion in micropores/mesopores of the coal matrix, and the adsorption−desorption kinetics of methane-coal. The model was verified with the results of the Langmuir isothermal adsorption equation at first. The conclusions were as follows:

(1) With a larger specific surface area of coal, the methane desorption-diffusion is faster. When there is a fixed volume of coal with a larger proportion of fractures, the initial adsorbed amount will be smaller. By hydraulic fracturing, the fractures of the coal reservoir will have a second development, which can effectively improve the specific surface area of coal and may make the pore connection better and the gas desorption-diffusion efficient.

(2) The flow and diffusion of methane are closely related to each other in the desorption-diffusion process. When the gas diffusivity is poor, the gas desorption can be effectively accelerated by increasing the drainage intensity, but when the gas diffusivity is good, increasing the flow velocity has little effect on the gas desorption. In productivity prediction or experiment, if the estimated gas diffusion coefficient is less than the order of $10^{-5}$ m$^2$/s, more attention should be paid to its accuracy; otherwise, the obtained results may have a large deviation from the real value.

(3) In the typical range of average pore sizes of coal, the gas desorption rate increases with the increase of pore size, and a larger affecting range of fracturing can greatly expand the average pore size. In addition, the low-rank coal with larger average pore size has more advantages in the process of methane desorption-diffusion. When the high-rank coal has a larger adsorbed amount and with the decrease of reservoir pressure, the low- and high-rank coals more easily desorb methane than medium-rank coal.

(4) In the kinetic study of the coalbed methane desorption-diffusion process, the accuracy of the obtained results may depend on the adsorption/desorption rate constant if the desorption rate constant is less than $10^6$ 1/s.

ASSOCIATED CONTENT

Supporting Information
The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acsomega.1c02499.

Appendix A The verification of the LB model (PDF)

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Notes
The authors declare no competing financial interest.
The data used to support the findings of this study are included in the article.

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