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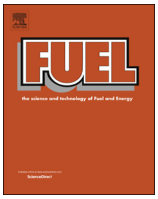

Full Length Article

Effects of surface roughness and derivation of scaling laws on gas transport in coal using a fractal-based lattice Boltzmann method

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ABSTRACT

Unconventional energy such as coal seam gas is trapped in a low porosity/permeability environment and poses challenges for production. Of particular interest is the mode of microscale gas transport through so-called coal cleats which form a network of micro-channels/fractures and allow for gas transfer through impermeable coal seams. The problem has attracted interest from many fields such as microstructural characterization, permeability-, porosity-, fluid flow-, diffusion-, adsorption/desorption- and adsorption-induced deformation studies. The main mode of gas flow is supported by the cleat network pattern for which the surface roughness is a very significant property of gas transport. Roughness plays an important role because adsorption is very sensitive to the change in the area. Direct studies on the effects of surface roughness for methane migration in coal by experimental methods are difficult to perform because the micro-scale heterogeneous pore structure and methane sorption properties are difficult to observe and therefore robust numerical simulations provide the most comprehensive method of investigation. In this paper, we develop a numerical model of coal seam gas diffusion and adsorption considering surface roughness based on fractal statistics and the lattice Boltzmann method. The rough surface is characterized by a 3D-Laser profiler and the fractal dimension of the cleat surface is quantified. Generic variants of the measured rough profiles are generated by the Weierstrass-Mandelbrot function through altering the fractal dimension D and length-scale parameter G. The fractal-based lattice Boltzmann method is introduced to solve the governing equations for the gas flow and diffusion processes and scaling laws may be a standardized analysis method and are applied for the non-dimensionalization of gas adsorption. By considering D ranging from 1.5 to 1.8 and G ranging from 1 to 20 it is found that the fractal dimension D has a small effect on the flow but a significant effect on the gas diffusion. In addition, the length-scale parameter G significantly affects gas transport through varying characteristic cleat aperture, and gas diffusion and adsorption by changing the contact area. The data rescaled by scaling laws provide a better analysis of gas adsorption through simplifying the assessment of the effects of multiple variables. Results of this work allow direct quantification of the effect of surface roughness on gas diffusion and adsorption in coal cleats and can provide an improved assessment of the effect of microscopic mechanisms of gas transfer/adsorption in coal on the overall large recovery of gas in the reservoir.

1. Introduction

Coal seam gas (CSG), or coal bed methane (CBM), is stored in underground coal seams. Its industrial production is largely controlled by the reservoir micro-structures and in particular the mechanism of adsorption/desorption on internal surfaces within the coal. Coal is a dual-porosity medium consisting of small internal pores within the matrix and macro-scale fracture or channels, called cleats [1–3]. Because of the distinctive structural character of coal, CSG recovery is commonly divided into two processes: gas transport in pores controlled by matrix diffusion and cleat network controlled by laminar flow. Many experimental and theoretical investigations have been done to study the mechanisms of CSG production in coal [4–9]. The traditional studies for methane transport assume that coal is homogeneous and consists of smooth-surface pores and fractures [10,11]. However, coal is a highly heterogeneous substance because a wide range of sizes of pores and cleats from nanometer to centimeter exist in coal [2]. This multiscale problem poses significant uncertainties for accurate assessments of the mechanism of methane storage and production. Theoretical models for methane production built upon the Fick's diffusion and Langmuir

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equations [12,13], neglect the importance of the kinetic gas migration mechanism in the coal's internal structure. However, the assessment of the gas migration mechanism is of primordial importance for the extraction of methane from coal seams. This paper introduces a numerical modeling framework for the investigation of the effects of rough surfaces on the methane transport mechanism by using a fractal-based lattice Boltzmann (LB) method.

To date, few models on the kinetic processes of gas diffusion and adsorption based on the pore-scale structure and cleat network in real coal are available. Gas diffusion and adsorption in coal have been studied since decades ago [14,15] and many research works have been published. Specifically, Thimons [14] and Smith [15] discussed the methane migration and predicted the gas content in coal with experimental and theoretical methods; Milewska-Duda proposed a theoretical model for descriptions of methane sorption isotherms in coal [5], and Pillalamarry studied the methane sorption and diffusion based on the Langmuir isotherm and Fick's Law for the evaluation of industrial production [1]. Assumptions made in the above studies are that coal is a homogeneous medium ignoring the cleat-matrix pattern. In the foregoing literature, methane adsorption has only been assumed to be affected by the local pressure–temperature conditions. To account for gas adsorption in a numerical model most researchers focused on the adsorption capacity of coal at pressure-temperature conditions [5,16,17], while adsorption rates received little attention. Exceptions are experimental studies on methane adsorption-diffusion modeled by Crank's approximation for the kinetic adsorption rate [12,18].

To the best of our knowledge, the kinetic effect of transport through the cleat-matrix system of coal has not been considered in previous studies. Gas flow through coal seams may, however, be significantly controlled by the methane adsorption in coal seams [9,19]. The cleat-matrix system also strictly affects the transport properties of gas through the coal seam. The release of methane from coal is a kinetic process in the coal matrix and cleat system, which is controlled by the topology of coal. Therefore, surface roughness as one of the topological properties may affect the gas diffusion and sorption. The effect of surface roughness on fluid flow, sorption and diffusion are well documented in Fluid Mechanics [20–22], Geophysics [23], Hydrology [24], Surface Science [25,26], carbon dioxide storage [27] and Heat Transfer [28], although a comprehensive assessment of all factors has not yet been available. It was found that the surface roughness plays a significant role in fluid flow and heat transfer. As 95% of methane is stored in coal by adsorption on internal surfaces [29], it is necessary to study the effects of surface roughness on the gas diffusion and adsorption. Scaling laws as a tool for interpreting the results have not yet been used and are introduced in this study. Numerical modeling of the kinetic gas migration through complex surfaces is an emerging tool, which is an ideal supplement to experimental techniques that do not allow the direct study of micro-processes on these internal mass transfer problems.

Conventionally, mathematical models have been built for gas transport by assuming fractures with flat surfaces and isotropic models for coal [11,30]. Nowadays, the microstructural data of the porous medium is available from advanced imaging techniques, such as 3D laser profiling [7], CT imaging [31], etc.. These techniques have set a new trend in Petroleum Engineering where investigations of microscopic mechanisms of oil and gas migration at the pore-scale level [32–34] are performed. However, the next step of numerical modeling post characterization has not yet found widespread applications in the discipline. We, therefore, use the data supplied by one of such characterization studies of a real coal cleat surface [7] for the next step of constructing a numerical model of gas transfer, diffusion, and adsorption on such a surface.

To this end, we use the surface roughness measurement described by fractal analysis. This analysis allows the determination of the fractal dimension and a length scale parameter. In this study, the Weierstrass-Mandelbrot (M-W) function is used to generate various rough surfaces by changing the fractal dimension and length-scale parameters. The simulations of methane diffusion and adsorption are run over the rough profiles built by the W-M function which are solved by the LB method as a result of its inherent kinetic nature. In this paper, a numerical model will, therefore, be developed to couple the two processes of methane diffusion and adsorption based on a fractal model with the LB method. This paper is divided into five sections. Section 2 introduces the building process of the fractal model of coal and the numerical method used in this work. Then, the results of the effects of fractal dimension, adsorption rate, and length-scale parameter on methane transport, and scaling laws for gas adsorption are presented in Section 3. The discussion is presented in Section 4. Finally, the conclusions are made in Section 5.

2. Mathematical models

2.1. Rough surface analysis

To analyze the fracture surface, the surface topography and roughness profiles are generally measured by stylus profilometers or laser profilometers. In this work, the data of the real rough surface of coal are provided by Dr. Gerami. The details of the coal sample can be found in this previous work [7]. The rough coal surface is extracted and scanned by a 3D laser profiler with a resolution of 0.5 nm in z-axis under laboratory conditions. A 3-D image of the scanned data is presented in Fig. 1.

Fractal dimension is an established method for characterization of surface roughness [35]. There are numerous algorithms available to calculate fractal dimension from the data obtained from profilers, such as Richardson plot [36], root-mean-square method [37], Hurst [38], box-counting [39], variogram or structure-function [40], and fast-Fourier transforms (FFT) analysis [41]. The variogram is simple to use, and relatively easy to interpret [40]. It is used in this paper for calculations of fractal dimension. The one-dimensional coal profile from the laser-scanned coal surface is presented in Fig. 2a with a corresponding fractal dimension of 1.89. The Weierstrass-Mandelbrot (W-M) fractal function, which is continuous and non-differentiable at all points, is used to describe the rough surface [42]. The expression of the function is given by

$$R(d) = G^{D-1} \sum_{i=n_1}^{\infty} \frac{\cos(2\pi\gamma^i d)}{\gamma^{i*(2-D)}}, 1 < \mathrm{D} < 2, \gamma \ > 1 \tag{1}$$

where G is a scaling constant, D is the fractal dimension of the surface profile and γ is the parameter determining the density of the spectrum and the relative phase differences between the spectral modes. A new surface profile is generated by Eq. (1) and shown in Fig. 2b. To verify the accuracy of the method, the variogram of the two profiles are compared and presented in Fig. 3a and b. The slopes of two fitting lines for original coal and generated profiles are 0.22 and 0.26, respectively. The corresponding fractal dimensions are 1.89 and 1.87 by the equation $D = 2 - \beta/2$ (β is the slop of variogram). The calculation error is acceptable.

2.2. Numerical model for CSG transport with the lattice Boltzmann method

The CSG transport in coal includes two processes that are the gas advection-diffusion in cleat networks and only diffusion in the coal matrix. This work focuses on the first process and considering the adsorption/desorption influence. The mechanism of advection-diffusion of CSG consists advection and diffusion section. Gas advection is driven by the gas velocity, and the diffusion part is controlled by the concentration gradient. The velocity distribution of gas in the coal cleat governed by Naiver-Stokes equations is solved by the lattice Boltzmann equation (LBE) with D2Q9 model [43,44], and the LB equations are expressed by