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Experimental study of the gas concentration boundary condition for diffusion through the coal particle

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ABSTRACT

Gas diffusion law for coal particles has been researched by many authors due to theoretical and practical significance to gas emission prediction and coal and gas outburst prevention. But its definition remains fuzzy for indeterminacy of the concentration boundary condition that mainly depends on the change rules of external gas pressure and temperature of the coal particles during the desorption process. In this paper, reliable data of the external gas pressure and temperature are obtained by using a self-developed experimental setup of which the most remarkable characteristic is the application of a specially-made real time data acquisition system capable of recording data at very short time intervals (several milliseconds). Experimental results showed that after the opening of pneumatic valve gas pressure decreased nonlinearly with increasing time, and gas pressure had exponent relation to time. Gas temperature decreased rapidly at first, then increased with a decreasing speed, and finally reached a constant. The final gas temperature did not rise to the initial equilibrium value. With increase of the equilibrium gas pressure, the lowest gas temperature decreased, and the temperature difference between the equilibrium gas temperature and the lowest gas temperature increased gradually. Based on the tested change rules of gas pressure and temperature, the concentration boundary condition is achieved.

1. Introduction and background

Coal is a complicated porous material. Large quantities of gas is stored in coal because the pores are so plentiful that just 1 cm^3 of coal can contain pores with an internal surface area of 3 m^2 (Moore, 2012). Gas mainly exists in states of adsorption or free. The adsorbed gas will be rapidly desorbed to free gas with the formation of broken coal during the normal coal mining and the abnormal coal and gas outburst processes (Czerw, 2011; Dutta et al., 2011). The high and irregular gas emissions lead to gas and ventilation problems in maintaining the necessary air quantities in ventilation systems to satisfy the statutory gas limitations for various coal production rates (Lunarzewski, 1998). And gas desorption is controlled by diffusion dynamics. Thus, gas emission estimation in coal mines requires a precise definition of gas diffusion law for coal particles. Besides, the gas diffusion law is important for determination of the lost gas which is a part of the gas content (a widely used index in coal and gas outburst proneness assessment) (Diamond and Schatzel, 1998; Wang et al., 2014). Thus, the gas diffusion law for the coal particles has been researched by many authors due to its theoretical and practical significance to gas emission prediction and coal and gas outburst prevention.

For the gas diffusion equation, gas transport in the coal particle is assumed to be concentration gradient-driven and is usually modeled by Fick's Second Law for spherically symmetric flow (Ni and San, 2000; Wang et al., 2012, 2014):

$$\frac{\partial c}{\partial t} = D\left(\frac{\partial^2 c}{\partial r^2} + \frac{2}{r}\frac{\partial c}{\partial r}\right) \tag{1}$$

where c is gas concentration; t is time; D is diffusion coefficient, which is supposed to be independent of concentration and location in coal particle; r is sphere radius. A schematic of the coordinate for gas diffusion through the coal particle is shown in Fig. 1.

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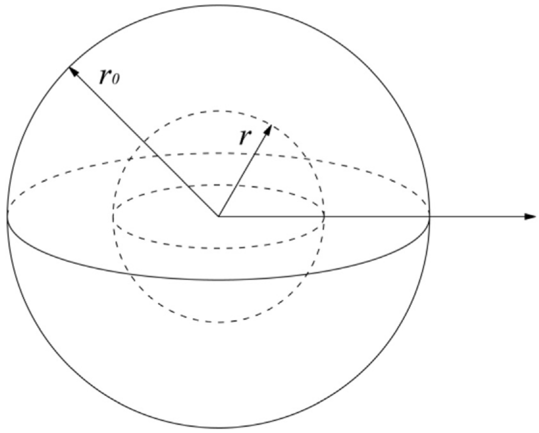

Fig. 1. Schematic of the coordinate for gas diffusion through the coal particle.

For the diffusion initial condition, it is considered that the gas concentration in coal is distributed equably when gas adsorption is in equilibrium. Then, the initial condition is always given:

$$c = c_0 \quad \text{at}(0 \le r \le r_0,\ t = 0) \tag{2}$$

where c_0 is the initial gas concentration which is regarded as a fixed value; r_0 is the diffusion path length (particle radius).

The boundary condition reflecting the relationship between gas concentration and time after coal particle is exposed to the atmosphere consists of two contents: one is at the center of coal particle, and the other is at the surface. There is unanimity on the former condition that is given:

$$c = c_1 \quad \text{at}(r = 0,\ t > 0) \tag{3}$$

where c_1 is gas concentration at the center of coal particle which is regarded as a fixed value.

However, many controversies exist in the designation of pressure and temperature variations for the latter condition resulting in three kinds of solutions to the Eq. (1):

(i) The isopiestic and isothermal boundary condition with a constant surface concentration given by Crank (1975) is:

$$c = c_2 \quad \text{at}(r = r_0,\ t > 0) \tag{4}$$

where c_2 is gas concentration at the coal particle surface which is regarded as a fixed value.

The corresponding relationship between desorbed gas and time can be expressed as:

$$\frac{V_t}{V_\infty} = 1 - \frac{6}{\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2}\exp\left[-\frac{Dn^2\pi^2 t}{r_0^2}\right] \tag{5}$$

where V_t is the desorbed volume at time t; V_∞ is the total desorbed volume.

This model assumes spherical, homogeneous coal particles of identical radius with smooth surfaces and is used to avoid complex mathematical calculations because of its simplicity (Busch and Gensterblum, 2011; Pillalamarry et al., 2011). But the precondition of constant surface concentration for Eq. (4) is always disputed, and changing external pressure is found by Clarkson and Bustin (1999); Busch et al. (2004), Cui et al. (2004), Siemons et al. (2007), and Czerw (2011).

(ii) Boundary condition proposed by Wang et al. (2012) based on the assumption of constant temperature and a linear decrease of external gas pressure is:

$$c = \frac{ab(p_0 - ht)}{1 + b(p_0 - ht)} \quad \text{at}(r = r_0,\ t > 0) \tag{6}$$

where p_0 is initial equilibrium gas pressure; h is pressure drop coefficient.

The corresponding analytical solution to the Eq. (1) is given as:

$$V_t = \frac{4}{3}\pi r_0^3\left[\frac{abp_0}{1 + bp_0} - \frac{ab(p_0 - ht)}{1 + b(p_0 - ht)}\right] - \frac{2abhr^3}{\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2}\int_0^t\frac{\exp\left[-Dn^2\pi^2(t-\tau)/r^2\right]}{\left[1 + b(p_0 - ht)\right]^2}d\tau \tag{7}$$

This boundary condition considers the external pressure variation and this is more conform to the fact. However, Eq. (6) is also questionable because of lack of clear evidence and laboratory data support for the assumption.

(iii) Ni and San (2000) and Nie et al. (2001) point that the external gas pressure and temperature will change with time with regard to gas exchange between coal matrix and pore. Based on this, the corresponding boundary condition is suggested:

$$-D\frac{\partial c}{\partial r} = \alpha\left(c - \frac{p}{RT}\right) \quad \text{at}(r = r_0,\ t > 0) \tag{8}$$

where α is convective mass transfer coefficient; p is external gas pressure; R is gas constant; T is external gas temperature.

The mathematical and physical model for gas diffusion through coal particle is founded and its analytical solution is obtained:

$$\frac{V_t}{V_\infty} = 1 - 6\sum_{n=1}^{\infty}\frac{(\beta_n\cos\beta_n - \sin\beta_n)^2}{\beta_n^2\left(\beta_n^2 - \sin\beta_n\cos\beta_n\right)}\exp\left(-\beta_n^2 Dt\Big/r_0^2\right) \tag{9}$$

where β_n is the root of $\tan\beta_n = \beta_n/\left(1 - \frac{\alpha r_0}{D}\right)$.

Compared with the former two kinds of boundary conditions, the one given by Eq. (8) is more accurate because of the considered time-varying gas pressure and temperature. But it is not yet well-enough defined because of the unclear change rules of external pressure and temperature.

In conclusion, according to the previous studies, descriptions and expressions of the diffusion equation and the initial condition are uniform, but the boundary condition for solving the diffusion equation is not finalized resulting in the non-uniform diffusion law. In this paper, reliable data of the external gas pressure and temperature are obtained by experiments, and their change rules are analyzed. Furthermore, the boundary condition is improved and completed based on the change rules. Thus, this work advances the research on the issue of gas diffusion through the coal particle. It is important for people to apply the diffusion law to gas emission prediction and coal and gas outburst prevention.

2. Experimental

2.1. Sample preparation

The coal was sampled in lumps from Xuehu coal mine of Shenhuo Coal and Power Group in Henan province, China. The coal