



A general solution and approximation for the diffusion of gas in a spherical coal sample



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ARTICLE INFO

Article history:

Received 10 October 2013

Received in revised form 15 November 2013

Accepted 8 December 2013

Available online 29 April 2014

Keywords:

Coal content

Lost gas

Spherical coal sample

Gas diffusion

Approximation

Error analysis

ABSTRACT

The square root relationship of gas release in the early stage of desorption is widely used to provide a simple and fast estimation of the lost gas in coal mines. However, questions arise as to how the relationship was theoretically derived, what are the assumptions and applicable conditions and how large the error will be. In this paper, the analytical solutions of gas concentration and fractional gas loss for the diffusion of gas in a spherical coal sample were given with detailed mathematical derivations based on the diffusion equation. The analytical solutions were approximated in case of small values of time and the error analyses associated with the approximation were also undertaken. The results indicate that the square root relationship of gas release is the first term of the approximation, and care must be taken in using the square root relationship as a significant error might be introduced with increase in the lost time and decrease in effective diameter of a spherical coal sample.

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1. Introduction

Gas content of coal is widely used in gas emission estimation, and gas outburst proneness assessment in underground coal mining [1]. The commonly used method for the estimation of the gas content is the direct desorption method. This method is based on observations of gas release from newly obtained samples, and typically involves extracting a coal sample, enclosing it in a sealed container and measuring the volume of gas released. With the direct method, the total gas content of a coal sample is made of three parts: lost gas, measurable gas, and residual gas [2–5]. The lost gas (Q_1) is the gas desorbed from the sample before it is placed in the canister. The measurable gas (Q_2) is the gas desorbed during transport and in the laboratory. The residual gas (Q_3) is the gas still contained in coal at one atmospheric pressure. While Q_2 and Q_3 can be directly measured, Q_1 has to be estimated.

The “lost gas” estimation method was firstly described by Bertard et al. [6]. It was stated in the paper that early in the desorption process the volume of gas released from coal was proportional to the square root of time. However no details were given as how the relationship was theoretically derived except mentioning that it was based on kinetics of gas desorption from coal. Since then this square root relationship has been widely used as a standard lost gas estimation method. The relationship has been found to be

significantly dependent on a number of factors such as sample shape, retrieval time, and physical character of the sample [7,8]. Crank did present in his book the analytical solutions of diffusion from cylindrical and spherical samples, but still no mathematical derivations were given [9]. This raises the questions: how the relationship was theoretically derived? What are the assumptions and applicable conditions and how large the error will be? To answer some of the questions and improve the accuracy of estimation, this paper gives detailed derivations of a general mathematical solution for the diffusion of gas in a spherical coal sample and an approximation solution. The detailed derivations of a general mathematical solution for the diffusion of gas in a cylindrical coal sample and an approximation solution have been published by the same group of authors of this paper [10]. These mathematical derivations also have particular relevance in determining the sorption time and diffusion coefficient in our numerical models of coal and gas outbursts [11,12].

2. Diffusion equation and the initial and boundary conditions

Gas release from coal is considered to be the process of diffusion in the coal matrix and desorption at surface. The diffusion through the matrix is assumed to be concentration gradient-driven and usually modeled using Fick's Second Law of Diffusion [13]. For a spherical sample with constant diffusion coefficient (D), the gas concentration (C) is dependent on the radial coordinate of the

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sphere (r) only, then the diffusion equation derived from Fick's Second Law of Diffusion is given as

$$\frac{\partial C}{\partial t} = D \left(\frac{\partial^2 C}{\partial r^2} + \frac{2}{r} \frac{\partial C}{\partial r} \right), \quad 0 \leq r < a, \quad t > 0 \tag{1}$$

The initial and boundary conditions can be expressed as:

$$C = C_0, \quad t = 0, \quad 0 \leq r < a \tag{2}$$

$$C = C_1, \quad r = a, \quad t > 0 \tag{3}$$

$$C = \text{finite}, \quad r = 0, \quad t > 0 \tag{4}$$

where a is the radius of the sphere; C_0 the initial uniform concentration; and C_1 the constant concentration at the surface of the sphere.

Let $u = Cr$, Eqs. (1)–(4) become

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial r^2} \tag{5}$$

$$u = rC_0, \quad t = 0, \quad 0 < r < a \tag{6}$$

$$u = aC_1, \quad r = a \tag{7}$$

$$u = 0, \quad r = 0 \tag{8}$$

Eqs. (5)–(8) can be analytically solved with either the method of separation of variables or the Laplace transform method. The latter approach is adopted in this paper because it is also used to derive approximations (Section 5 of this paper) of the general solutions.

3. General solution

3.1. Solution of gas concentration

Application of the Laplace transform to Eq. (5) leads to the subsidiary equation

$$\frac{\partial^2 \bar{u}}{\partial r^2} - q^2 \bar{u} = -\frac{rC_0}{D}, \quad 0 \leq r < a \tag{9}$$

With the conditions

$$\bar{u} = \frac{aC_1}{p}, \quad r = a \tag{10}$$

$$\bar{u} = 0, \quad r = 0 \tag{11}$$

where $\bar{u} = \int_0^\infty e^{-pt} u dt$ is the Laplace transform of u , $q^2 = p/D$, p is the Laplace variable.

The solution of Eqs. (9)–(11) is given as

$$\begin{aligned} \bar{u} &= \frac{a(C_1 - C_0)(e^{qr} - e^{-qr})}{p(e^{qa} - e^{-qa})} + \frac{rC_0}{p} \\ &= \frac{a(C_1 - C_0) \sinh(qr)/q}{p \sinh(qa)/q} + \frac{rC_0}{p} \end{aligned} \tag{12}$$

By applying the method Laplace transform of partial function, the inversion of the Laplace transform of Eq. (12) is obtained as

$$u = rC_1 + \frac{2a(C_1 - C_0)}{\pi} \sum_{n=1}^\infty \frac{(-1)^n}{n} \sin \frac{n\pi r}{a} \exp \left(-\frac{Dn^2\pi^2 t}{a^2} \right) \tag{13}$$

We then have

$$C = C_1 + \frac{2a(C_1 - C_0)}{\pi r} \sum_{n=1}^\infty \frac{(-1)^n}{n} \sin \frac{n\pi r}{a} \exp \left(-\frac{Dn^2\pi^2 t}{a^2} \right) \tag{14}$$

or

$$\frac{C - C_0}{C_1 - C_0} = 1 + \frac{2a}{\pi r} \sum_{n=1}^\infty \frac{(-1)^n}{n} \sin \frac{n\pi r}{a} \exp \left(-\frac{Dn^2\pi^2 t}{a^2} \right) \tag{15}$$

3.2. Solution of the fractional loss

Let the total gas volume in the sample at time t be Q , we then have

$$\begin{aligned} Q &= \int_0^a C \cdot 4\pi r^2 dr \\ &= \frac{4\pi a^3}{3} C_1 - \frac{8a^3(C_1 - C_0)}{\pi} \sum_{n=1}^\infty \frac{1}{n^2} \exp \left(-\frac{Dn^2\pi^2 t}{a^2} \right) \end{aligned}$$

At $t = 0$, the initial total concentration is $Q_0 = \frac{4\pi a^3}{3} C_0$, the total desorbed gas M_t until time t is

$$\begin{aligned} M_t &= Q_0 - Q \\ &= \frac{4\pi a^3}{3} (C_0 - C_1) + \frac{8a^3(C_1 - C_0)}{\pi} \sum_{n=1}^\infty \frac{1}{n^2} \exp \left(-\frac{Dn^2\pi^2 t}{a^2} \right) \end{aligned}$$

At $t = \infty$, we have M_∞ as follows

$$M_\infty = \lim_{t \rightarrow \infty} M_t = \frac{4\pi a^3}{3} (C_0 - C_1) \tag{16}$$

Thus we obtain the fractional loss as

$$\frac{M_t}{M_\infty} = 1 - \frac{6}{\pi^2} \sum_{n=1}^\infty \frac{1}{n^2} \exp \left(-\frac{Dn^2\pi^2 t}{a^2} \right) \tag{17}$$

4. Convergence analysis

Although Eq. (17) is an analytical solution, it contains an infinite number of exponential terms. In practical applications, it is necessary to cut off to a finite number of terms. To do this, the convergence of Eq. (17) needs to be studied. If we set the cut-off error to be $10^{-2} \times \sqrt{Dt}/a$ the minimum number of terms required to obtain this precision can be calculated. Fig. 1 shows the variation of this minimum number of terms with Dt/a^2 . It can be seen that with the decrease of Dt/a^2 value, the minimum number of terms required to obtain this precision increases dramatically. Therefore, Eq. (17) converges rapidly for large values of time, for short times (t close to zero), the number of terms required to calculate the fractional loss accurately increases rapidly. This is the reason why the approximation of Eq. (22) (in Section 5 of this paper) is generally used instead in practical estimation of the lost gas in the earlier stage of desorption.

5. Approximations of the general solutions

In the case of small values of time the general solutions Eqs. (15) and (17) can be approximated as follows.

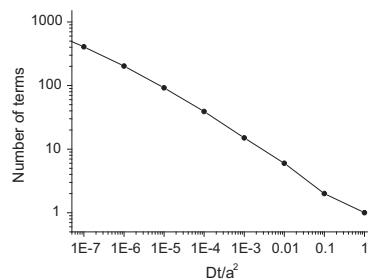


Fig. 1. Minimum number of terms required to make Eq. (17) converge versus Dt/a^2 .

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