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Gas diffusion in a cylindrical coal sample – A general solution, approximation and error analyses

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ABSTRACT

The analytical mathematical solutions of gas concentration and fractional gas loss for the diffusion of gas in a cylindrical coal sample were given with detailed mathematical derivations by assuming that the diffusion of gas through the coal matrix is concentration gradient-driven and obeys the Fick's Second Law of Diffusion. 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 in the early stage of desorption, which is widely used to provide a simple and fast estimation of the lost gas, 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 cylindrical coal sample.

1. Introduction

Gas content in a coal seam is commonly used in coal mine safety such as gas emission control and gas outburst control as well as coal seam methane resource assessment and recovery applications. The gas content is usually measured with either an indirect method or a direct method. The indirect method is based on empirical correlations or laboratory derived sorption isotherm gas storage capacity data. The direct method is based on observations of gas release from newly obtained samples, and it typically involves extracting a coal sample (often core sample), enclosing it in a sealed container and measuring the volume of gas released. As the direct method provides a fast in situ estimation of gas content, it is widely used in the coal industry and coal seam gas industry. With the direct method, the total gas content of a coal sample is made of three parts: lost gas, measurable gas, and residual gas [1–5]. The lost gas (Q_1) is the gas lost from the sample, subsequent to its being removed from its in situ position and prior to its containment in an airtight desorption canister. The measurable gas (Q_2) is the gas desorbed at atmospheric pressure from the non-pulverized coal sample. 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 Q_1 estimation method was firstly described in a paper written 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, which is indicated by US Report of Investigation 7767 (1973), Australian Standard AS 3980-1999 (1999) and Standards of China (2009) [7–9]. However, the relationship has been found to be significantly dependent on a number of factors such as sample retrieval time, physical character of the sample, and the type of drilling fluid [10,11]. This raises the questions of how the relationship was theoretically derived, its validity, its applicable conditions, and its error.

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 cylindrical coal, an approximation solution, error analyses of the approximation and its application in the Q_1 estimation.

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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 the Fick's Second Law of Diffusion [12]. For a cylindrical sample, if one assumes that the cylinder length is infinite, diffusion coefficient (D) is constant, and the gas concentration (C) depends on the radial coordinate of the cylinder (r) only, then the diffusion equation derived from the Fick's Second Law of Diffusion is given as

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

The initial and boundary conditions can be expressed as:

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

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

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

where a is the radius of the cylinder; C_0 the initial uniform concentration; and C_1 the constant concentration at the surface of the cylinder. Eq. (1) 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 of the general solutions.

3. General solution

3.1. Solution of gas concentration

Application of the Laplace transform to Eq. (1) leads to the subsidiary equation:

$$\frac{d^2\overline{C}}{dr^2}+\frac{1}{r}\frac{d\overline{C}}{dr}-q^2\overline{C}=-\frac{C_0}{D}(0\le r<a) \tag{5}$$

with the conditions

$$\overline{C}=C_1/p \quad (r=a) \tag{6}$$

$$\overline{C}=\text{finite} \quad (r=0) \tag{7}$$

where $\overline{C}=\int_0^\infty e^{-pt}Cdt$ is the Laplace transform of C; $q^2=p/D$; and p the Laplace variable.

Eq. (5) is a modified Bessel equation which has two general solutions: $I_0(qr)$ and $K_0(qr)$, where $I_0(x)$ and $K_0(x)$ are respectively modified Bessel functions of the first and second kinds. As $r\to 0$, $K_0(qr)\to\infty$, it has no physical meanings and is discarded. Therefore the solution of Eqs. (5)–(7) can be given as:

$$\overline{C}=\frac{(C_1-C_0)}{p}\frac{I_0(qr)}{I_0(qa)}+\frac{C_0}{p} \tag{8}$$

To obtain the inversion of the Laplace transform of Eq. (8), the method of Laplace transform of partial function is used. Here $f(p)=I_0(qr)$, $g(p)=pI_0(qa)$ and $g'(p)=I_0(qa)+aqI_1(qa)/2$, where $f(p)$ and $g(p)$ are polynomials in p. We need to find the zeros of $g(p)=0$ which consists of two parts: $p=0$ and $I_0(qa)=0$.For the zero $p=0$, we have $g'(p)=1$, $f(p)=I_0(0)=1$, so the contribution of this term to C is C_1-C_0. The other zeros of $I_0(qa)$ are at $p=-D\alpha_n^2$, where $\pm\alpha_n$, $n=1, 2, 3, \ldots$, are the roots of $I_0(a\alpha)=0$.Using the property of the Bessel functions, we have $g'(p)|_{q=i\alpha_n}=i\alpha_n aI_1(i\alpha_n a)/2=i\alpha_n aiJ_1(\alpha_n a)/2=-a\alpha_n J_1(\alpha_n a)/2$, the contribution of $p=-D\alpha_n^2$ (or $q=i\alpha_n$) to C is

$$(C_1-C_0)\sum_{n=1}^{\infty}\frac{\exp(-D(\alpha_n^2 t)I_0(i\alpha_n r)}{-a\alpha_n J_1(\alpha_n a)/2}$$

Using the property of the Bessel functions again, we have $I_0(i\alpha_n r)=J_0(\alpha_n r)$. Therefore we obtain the inversion of the Laplace transform of C as follows:

$$C=C_1-\frac{2(C_1-C_0)}{a}\sum_{n=1}^{\infty}\frac{\exp(-D\alpha_n^2 t)J_0(\alpha_n r)}{\alpha_n J_1(\alpha_n a)} \tag{9}$$

or

$$\frac{C-C_0}{C_1-C_0}=1-\frac{2}{a}\sum_{n=1}^{\infty}\frac{\exp(-D\alpha_n^2 t)J_0(\alpha_n r)}{\alpha_n J_1(\alpha_n a)} \tag{10}$$

where $J_0(x)$ is the Bessel function of the first kind of order zero; and $J_1(x)$ the Bessel function of the first order, α_n, $n=1, 2, 3, \ldots$, are roots of

$$J_0(\alpha a)=0 \tag{11}$$

3.2. Solution of the fractional loss

Let the total gas volume in the sample at time t be Q, that is, $Q=\int_0^a C\cdot\pi r^2 dr$, and assume that $\overline{Q}$ is the Laplace transform of Q. Using the derivative of the Bessel functions, we obtain:

$$\overline{Q}=\frac{2\pi a(C_1-C_0)}{p}\frac{I_1(qa)/q}{I_0(qa)}+\frac{\pi a^2 C_0}{p} \tag{12}$$

Again we use the method of Laplace transform of partial function to obtain the inversion of the Laplace transform. Here $f(p)=I_1(qa)/q$, $g(p)=pI_0(qa)$, and $g'(p)=I_0(qa)+aqI_1(qa)/2$. For the zero $p=0$, $g'(p)=1$, $f(p)=\lim_{q\to 0}I_1(qa)/q=a/2$. So the contribution of this term to Q is $\pi a^2(C_1 - C_0)$. The other zeros of $I_0(qa)$ are at $p=-D\alpha_n^2$, where $\pm\alpha_n$ are the roots of $I_0(a\alpha)=0$ and $n=1, 2, 3, \ldots$

By applying the property of the Bessel functions, we have $g'(p)|_{q=i\alpha_n}=i\alpha_n aI_1(i\alpha_n a)/2=i\alpha_n aiJ_1(\alpha_n a)/2=-a\alpha_n J_1(\alpha_n a)/2$ and $f(p)=I_1(i\alpha_n a)/i\alpha_n=J_1(\alpha_n a)/\alpha_n$. Then the contribution of $p=-D\alpha_n^2$ (or $q=i\alpha_n$) to Qis $-4\pi(C_1-C_0)\sum_{n=1}^{\infty}\frac{\exp(-D\alpha_n^2 t)}{\alpha_n^2}$. Therefore we obtain:

$$Q=\pi a^2 C_1-4\pi(C_1-C_0)\sum_{n=1}^{\infty}\frac{\exp(-D\alpha_n^2 t)}{\alpha_n^2} \tag{13}$$

At $t=0$, the initial total concentration is $Q_0=\pi a^2 C_0$. The total desorbed gas M_t at time t is

$$M_t=Q_0-Q=\pi a^2(C_0-C_1)+4\pi(C_1-C_0)\sum_{n=1}^{\infty}\frac{\exp(-D\alpha_n^2 t)}{\alpha_n^2}$$

At $t=\infty$, the total gas that may be released is:

$$M_\infty=\lim_{t\to\infty}M_t=\pi a^2(C_0-C_1) \tag{14}$$

Thus we obtain the fractional loss as

$$\frac{M_t}{M_\infty}=1-\sum_{n=1}^{\infty}\frac{4}{\alpha_n^2 a^2}\exp(-D\alpha_n^2 t) \tag{15}$$

4. Convergence analysis of the fractional loss

Although Eq. (15) is an analytical solution, it contains infinite number of exponential terms with the roots of Bessel function involved. In practical applications, one has to cut off to finite number of terms. To do this, the convergence of Eq. (15) 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 the value of Dt/a^2. As can be seen in Fig. 1, with the decrease