

METHANE DESORPTION AS A SOURCE OF GAS FLOW IN COAL BEDS

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Desorption exhibited by the diffusion from micropores (of the matrix) to macropores (fractures) system occurs in dual porosity coal system due to the drainage process in coal beds. Gas in the micropores, close to the fractures is in equilibrium with a free gas, volume of which depends on the pressure in micropores. This dependence fits in with Langmuir's theory of adsorption isotherms. To estimate the volume of gas adsorbed in the micropores far from fractures, a model of quasi-steady state has been used. This model is based on the first-order kinetics equation. The author demonstrates how to interpret the desorption source formula of mass balance in physical terms. The role of diffusivity in delayed gas supply is pointed out. The desorption source in the micropore gas flow model is presented in the characteristic form of integral. Numerical integration in successive time steps of coal bed methane production has been performed. In this way the formula for the discharge of adsorbed gas has been obtained.

Key words: gas flow, kinetics, desorption, coal

Notation

- D – micropore diffusion coefficient [m^2/s]
- α – diffusivity [$1/\text{s}$]
- t – time [s]
- T_d – characteristic sorption time [s]
- T_f – characteristic time of the gas flow through the fractures [s]

- p - macropore pressure of gas [Pa]
 V - volume of gas currently adsorbed in micropores [m^3/kg]
 V_E - volume of adsorbed gas in equilibrium with free gas [m^3/kg]
 V_m - Langmuir's isotherm sorption constant [m^3/kg]
 b - Langmuir's isotherm pressure constant [1/Pa]
 k - effective permeability to gas [1 darcy= 10^{-12}m^2]
 μ - gas viscosity [Pa·s]
 Z - real-gas deviation factor
 φ - macropore porosity
 C_g - gas compressibility [1/Pa]
 C_s - sorption compressibility [1/Pa]
 T - temperature [K]

Subscripts

- g - gas
 sc - standard conditions
 n - index of time step

1. Introduction

A major portion of gas stored in coal beds exists in an adsorbed state rather than as free gas. The coal beds reveal a dual-porosity nature, i.e. they contain both the low-permeability high storage primary porosity system (micropores) and the low-storage high-permeability secondary porosity system (macropores). Although the diameters and apertures characteristic for both the systems may vary within a wide range, yet Darcy's flow may occur only in the system of cleats and fractures. On the other hand gas may be adsorbed in the system of micropores both on the surface of coal and absorbed within the molecular coal volume.

When the pressure in the coal macropores is reduced, gas desorbs from the coal matrix. This may be accompanied by a prior influx of water from the exploitation wells. As the reservoir pressure is lowered, gas is desorbed and saturation with free gas in macropores is increased until the gas starts to move in the fractures (increase in the gas relative permeability and decrease in the water relative permeability). Thus the desorption of gas from the coal

matrix is followed by the flow through fractures.

The initial state in coal beds is followed by a transient state with the characteristic maximum of the gas rate. Then the discharge of gas is controlled by the desorption process. Duration of this interval depends on whether the desorption is fast or slow, which is determined by the time constant α of gas release being the inverse of the characteristic sorption time T_d .

In the subsequent time interval the coal bed with exploitation wells is in a quasi-steady state. The characteristic time T_f of the flow of gas through fractures is the time required for a well to reach this state.

In some cases, occasionally admit in practice, when the release of the absorbed gas is slow, a kind of delay with the definite time constant a of degasification process of the coal bed takes place.

For engineering purposes the gas production can be represented by a mathematical model focussed on the process dominating here. The above mentioned delay should be introduced into this model in an explicit form and discharge of the desorbed gas has to be estimated.

2. The role of desorption in considered problem simulations

Several models have been developed to simulate the coal bed methane. These models differ in description of the process of methane desorption and the flow through the macropore system. There may be two-stage systems of coal bed drainage or one-stage systems for degasification of the dry coal beds.

It is often assumed that Darcy's flow is observed in macropores, while the flow in micropores is governed by the diffusion resulting from the desorption process. This refers in particular to the coal beds deposited deeper. In coal mines where the sorptive properties of coal give prompt release of methane and the characteristic time of desorption T_d is short, a preferable characteristic time required for reaching the quasi-steady state T_f should not be too long.

The time T_d which is the inverse of diffusivity α depends on the effective diffusion coefficient D and on the geometrical parameter R of matrix grains in the micropore structure of coal.

The diffusivity values $\alpha = D/R^2$ are determined by direct methods (cf Diamond and Levin (1981), Smith and Williams (1984)), as well as the indirect ones (cf Ruppel et al. (1974)). Seidle (Metcalf et al. (1992)) and other researchers recommend the following formula for the time interval T_d [s] to

be applied in the direct methods

$$\mathcal{T}_d \cong \frac{9.5}{\alpha} \quad (2.1)$$

In the simulation carried out by Metcalfe et al. (1992), as well as in the calculations presented by Seidle and Arri (1990), the sorptive properties typical for San Juan Basin were used. On the whole, they are characterized by high diffusivity of coal, which, moreover, exhibits considerable permeability. The time required to reach the quasi-steady state by a coal bed with a well has been estimated by these authors as $\mathcal{T}_d = 1270$ hours. Only the characteristic times of desorption $\mathcal{T}_d = 0.2, 2$ and 20 days respectively, were used for the present simulation. These values as well as all higher ones did not change relatively prompt attaining of the peak gas rate and did not affect the production of gas. Only in coal beds with high diffusivity and considerable permeability the time required for attaining a quasi-steady state is considerably longer than the characteristic time of sorption ($\mathcal{T}_f \ll \mathcal{T}_d$).

In the cases of very prompt gas release from the matrix (micropore system) the kinetics of desorption may not be taken into consideration for engineering purposes, which, within the limits $\alpha \rightarrow \infty$, corresponds to immediate establishing of the equilibrium state between the gas released from the matrix and free gas at a given pressure in the fractures. As the mass balance in the model of such a flow has already been described in literature, only the formula for equilibrium sorption isotherm of sorption source q_s is taken into consideration

$$q_s = \frac{\partial V_E}{\partial t} = V_m \frac{b}{(1 + bp)^2} \frac{\partial p}{\partial t} \quad (2.2)$$

and therefore

$$\nabla \cdot \left(\frac{k_g p}{Z \mu_g} \nabla p \right) = \varphi C_g \frac{p}{Z} \frac{\partial p}{\partial t} + \frac{p_{sc} V_m T b}{Z_{sc} T_{sc} (1 + bp)^2} \frac{\partial p}{\partial t} \quad (2.3)$$

In Eqs (2.2) and (2.3) Langmuir's isotherm has been used and the equation of flow (2.3) has been given above only to point out the role of the source of gas desorption.

The coefficient at the source term occurring in Eq (2.3) is included in the sorption compressibility

$$C_s = \frac{p_{sc} Z T}{p Z_{sc} T_{sc}} V_m \frac{b}{\varphi (1 + bp)^2} \quad (2.4)$$

In coal beds where the sorption conditions are difficult and diffusion process in the system of micropores lasts for a long time, the time \mathcal{T}_f of attaining

the quasi-steady state is also long. The long time \mathcal{T}_f for gas flow in fractures typical for some coal wells is primarily due to large sorption compressibility C_s . Such conditions are probably found in Mary Lee Group of beds in Warrior Basin (Alabama), where King and Ertekin (1988) estimated the time $\mathcal{T}_d \cong 2 \cdot 10^7$ s. Such a value is consistent with this evaluated with the formula for estimating of characteristic desorption time given by Remner et al. (1986)

$$\mathcal{T}_d \cong \frac{1}{\alpha} = \frac{R^2}{D} \quad (2.5)$$

Also a small value of the diffusion coefficient D and slow desorption are characteristic for coal in Lower Silesian Coal Basin (Poland), which, moreover, shows extremely low permeability: $k \cong 10^{-3}$ mDarcy, which has been established on the basis of in situ investigations based on an appropriate method (cf Olajossy (1987)).

For a limited rate of gas release from micropores the desorption kinetics is essential. At times, the equation representing the kinetics is simplified as follows

$$\frac{\partial V}{\partial t} = \alpha(V_s - V) \quad (2.6)$$

where $V_s = \text{const}$ denotes the saturation volume of adsorbed gas and V denotes the volume of gas currently adsorbed in micropores. This equation may be important when methane is released from coal exposed to atmosphere. Thus Eq (2.6) might be applied to description of the experimental investigations (cf Yalcin and Durucan (1991)) referring to broken coal gas emission.

King and Ertekin (1988) proposed a model including a non-steady state desorption term. An implicit assumption accepted in this model is that the adsorbed gas is not necessarily in equilibrium with the free gas. King and Ertekin (1988) assumed that gas in micropores adhering closely to the fractures is in equilibrium with the free gas. For gas adsorbed in the micropores distant from the fractures the model of first-order kinetics has been used

$$\frac{\partial V}{\partial t} = \alpha [V_e(p_g) - V] \quad (2.7)$$

Thus the difference between the gas volume in the transient equilibrium in macropores and that absorbed in micropores is essential.

Moreover, it King and Ertekin (1988) assumed that the volume of adsorbed gas in the transient equilibrium with the free gas can be represented by means of Langmuir's isotherm

$$V_E = V_m \frac{bp}{1 + bp} \quad (2.8)$$

Besides Eqs (2.7) and (2.8) the model contains an equation for gas flow

$$\nabla \cdot \left(\frac{k_g p}{\mu_g Z} \nabla p \right) = \frac{p_{sc} T}{T_{sc}} \frac{\partial V}{\partial t} + \frac{\varphi C_g p}{Z} \frac{\partial p}{\partial t} \quad (2.9)$$

This model has been extended to comprise simulation of the two-stage flow including water by King and Ertekin (1988), where the finite differences method has been used to solve these problems.

Further on, there will be presented a flow equation equivalent to Eq (2.9) where two stages of gas desorption from the micropore system will be explicitly identified. They will result from the adopted kinetics model (2.7). A method of numerical calculation of the discharge of gas desorption will be also given.

3. Delayed yield of gas from the coal matrix

Here in after we will try to give a more fundamental, physico-chemical meaning to the model based on Eqs (2.7) \div (2.9).

In some cases, significant lowering of the free gas and water pressure may occur before the equivalent sorption pressure has been reached and the adsorbed gas has been released.

If this time moment is arbitrarily adopted as the beginning, $t = 0$, when $V_E = 0$, then in the subsequent time interval T an almost instantaneous release of the gas adsorbed in the micropores close to the fractures in easily accessible adsorption centres will take place. Then, in the time interval ΔT the volume of the released gas will be equal to ΔV_E .

During the next time interval $t > T$ a delayed yield of the absorbed gas from the coal matrix will occur. Then the gas volume increases relatively by $\Delta V_E \exp[-\alpha(t-T)]$. The cumulative volume of gas V_{cum} in both the intervals amounts to

$$\int_0^T \frac{\partial V_E}{\partial t} dt + \int_T^\infty \frac{\partial V_E}{\partial t} e^{-\alpha(t-T)} dt = V_{cum} \quad (3.1)$$

An interesting relation can be obtained from the desorption kinetics equation (2.7). To obtain it we need only to multiply both sides of this equation by $e^{\alpha t}$

$$\frac{dV}{dt} e^{\alpha t} + \alpha V e^{\alpha t} = \alpha V_E e^{\alpha t} \quad (3.2)$$

The left-hand side of this equation is derivative of the term $Ve^{\alpha t}$, hence

$$Ve^{\alpha t} = \int \alpha V_E e^{\alpha t} dt \quad (3.3)$$

By integrating by parts within the time limits from zero to an arbitrary moment t , we obtain

$$V_E - V = \int_0^t \frac{\partial V_E}{\partial t} e^{-\alpha(t-\tau)} d\tau \quad (3.4)$$

As a result, the kinetics equation will now assume a form equivalent to Eq (2.7), but explicitly revealing the delayed gas supply (for $t > \tau$)

$$\frac{\partial V}{\partial t} = \alpha \int_0^t \frac{\partial V_E}{\partial t} e^{-\alpha(t-\tau)} d\tau \quad (3.5)$$

In this way the equation of gas flow (2.9) will take on the equivalent form

$$\nabla \cdot \left(\frac{k_g}{\mu_g Z} p \nabla p \right) = \frac{\varphi C_g}{Z} p \frac{\partial p}{\partial t} + \frac{p_{sc} T}{T_{sc}} \alpha \int_0^t \frac{\partial V_E}{\partial t} e^{-\alpha(t-\tau)} d\tau \quad (3.6)$$

where V_E , similarly as the pressure p , may be controlled in a system of macropores.

It is thus a form entirely equivalent to that of the equation for gas flow, without changing essentially the previous model for degasification to which there may be added the equation of water flow and the corresponding conditions for coal bed drainage. The source term in Eq (3.6) will be used to determine the discharge of gas desorption. However, the method applied to this estimation will differ from that found in the known so far models the degasification of coal seams.

4. Algorithm for determination of the amount of desorbed gas

Let us denote by I_n the integral in the solution of Eq (3.4)

$$I_n = \int_0^{t_n} \frac{\partial V_E}{\partial t} e^{-\alpha(t_n-\tau)} d\tau \quad (4.1)$$

and by I_{n+1} the integral

$$I_{n+1} = \int_0^{t_{n+1}} \frac{\partial V_E}{\partial t} e^{-\alpha(t_{n+1}-\tau)} d\tau \quad (4.2)$$

where $t_{n+1} - t_n = \Delta t$.

From which it is seen that

$$I_{n+1} = I_n e^{-\alpha \Delta t} + I_{n,n+1} \quad (4.3)$$

where

$$I_{n,n+1} = e^{-\alpha(t_n + \Delta t)} \int_{t_n}^{t_{n+1}} \frac{\partial V_E}{\partial t} e^{\alpha \tau} d\tau \quad (4.4)$$

As a result of the assumed continuity and boundedness of derivative $\partial V_E / \partial t$, and substitution of this derivative with the finite difference within small limits (t_n, t_{n+1})

$$\frac{\partial V_E}{\partial t} \cong \frac{V_{E,n+1} - V_{E,n}}{\Delta t}$$

following several simple transformations of the right-hand side of Eq (4.4), we obtain

$$I_{n+1} = I_n e^{-\alpha \Delta t} + \frac{1}{\alpha \Delta t} (V_{E,n+1} - V_{E,n}) (1 - e^{-\alpha \Delta t}) \quad (4.5)$$

In this way we may write numerical expressions for integrals in the successive time steps ($n = 0, 1, 2, \dots, N$).

Representing now the solution (3.4) as

$$V_{E,n+1} - V_{n+1} = I_{n+1} \quad (4.6)$$

and utilizing Eq (4.5), since also $I_n = V_{E,n} - V_n$, we get

$$V_{n+1} = V_{E,n+1} - (V_{E,n} - V_n) e^{-\alpha \Delta t} - \frac{1}{\alpha \Delta t} (V_{E,n+1} - V_{E,n}) (1 - e^{-\alpha \Delta t}) \quad (4.7)$$

Hence, on the basis of the calculated gas volume V_n at the time step n , it is possible to calculate the amount of gas V_{n+1} at the subsequent $(n + 1)$ step.

The form of Eq (4.7) is very characteristic for some dynamical systems supplied with a delayed source. For instance, analogical situation arises in hydrogeology, when we consider infiltration to the underground water magazine from another layer through a semi-permeable layer.

In the considered case, the delayed infiltration is replaced with slow desorption of gas from inside the coal matrix.

By defining the discharge of gas desorption as a change in volume in the time interval Δt

$$q_n = \frac{V_{n+1} - V_n}{\Delta t} \quad (4.8)$$

we obtain ultimately

$$q_n = \frac{1}{\Delta t} \left[V_{E,n+1} - V_n - (V_{E,n} - V_n)e^{-\alpha\Delta t} - \frac{1}{\alpha\Delta t} (V_{E,n+1} - V_{E,n}) (1 - e^{-\alpha\Delta t}) \right] \quad (4.9)$$

It may be noticed that the value of time constant α , as well as the time step Δt have a significant effect on the volume of temporary gas discharge for an arbitrary n . The cumulated amount of the desorbed gas is

$$Q_c = \sum_{n=0}^N q_n (t_{n+1} - t_n) \quad (4.10)$$

The main aim of this paper has been reached with derivation of Eq (4.9).

5. Additional remarks

Eq (4.9) defining the desorption discharge is valid for the entire time of degasification of a coal bed. King et al. (1986) supplied a simplified method for determining the discharge of gas desorption. When integrating the kinetics equation (2.7), in order to simplify the procedure, it has been assumed that the volume of gas in equilibrium with free gas is a constant measured at the midpoint of a time interval. The equation obtained that way is as follows (cf King and Ertekin (1988))

$$q_n = \frac{1}{\Delta t} \left[\frac{1}{2} (1 - e^{-\alpha\Delta t}) (V_{E,n+1} + V_{E,n}) - (1 - e^{-\alpha\Delta t}) V_n \right] \quad (5.1)$$

In both extreme cases: immediate gas release $\alpha \rightarrow \infty$ and very slow desorption $\alpha \rightarrow 0$, Eqs (4.9) and (5.1) give similar asymptotic values of gas discharge.

However, the case: $\alpha \rightarrow \infty$, that is $T_d \rightarrow 0$, is not very interesting, particularly with reference to Polish coal basins, which are usually characterized with a reverse trend, i.e. very low diffusivity, that is very high value of the characteristic time of T_d desorption.

Under the conditions of very slow desorption we may quote the value $\alpha \approx 10^{-8} \text{ s}^{-1}$, so that $\alpha\Delta t \ll 1$. Therefore, the comparative analysis of

Eqs (4.9) and (5.1) allows us to expand the function $\exp(-\alpha\Delta t)$ into a series, obtaining for Eq (4.9)

$$q_n \cong \frac{1}{\Delta t} (V_{E,n+1} - V_n) \frac{\alpha\Delta t}{1 + \alpha\Delta t} \quad (5.2)$$

and for Eq (5.1)

$$q_n^* \cong \frac{1}{\Delta t} \left[\frac{1}{2} (V_{E,n+1} + V_{E,n}) - V_n \right] \frac{\alpha\Delta t}{1 + \alpha\Delta t} \quad (5.3)$$

respectively.

And hence, as for an arbitrary n

$$\frac{1}{2} (V_{E,n+1} + V_{E,n}) < \frac{1}{2} (V_{E,n+1} + V_{E,n+1}) = V_{E,n+1}$$

it is clear that under such conditions, Eq (4.9) provides higher values of q_n desorption discharge than Eq (5.1). It is justified with the above mentioned effect of the delayed yield of adsorbed gas resulting in slow desorption, which has been taken into consideration when derivating Eq (4.9).

Unfortunately, as the results of experimental investigations of the desorption relevant to the conditions described above have not been reached so far, it seems that further analysis of this problem is not necessary.

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Desorpcja metanu jako źródło przepływu gazu w pokładach węgla

Streszczenie

W systemie podwójnej porowatości węgla wskutek drenażu pokładu następuje desorpcja, która objawia się dyfuzją z mikroporów matrycy do systemu makroporów (szczelin). Gaz w mikroporach przyległych do szczelin jest w równowadze z gazem wolnym, którego objętość zależy od ciśnienia w makroporach. Tę zależność przyjęto według teorii Langmuira dla izotermy adsorpcji. Natomiast do oceny ilości gazu adsorbowanego w mikroporach dalekich od szczelin użyto modelu quasi-ustalonego. Model ten oparty jest na równaniu kinetyki pierwszego rzędu.

W pracy pokazano, jak fizycznie należy interpretować wyrażenie opisujące źródło desorpcji w równaniu przepływu gazu. Wskazano przy tym na rolę dyfuzyjności w opóźnionym dostarczaniu gazu z matrycy do systemu szczelin. Wyraz źródła desorpcji ma charakterystyczną postać całki w stosowanym modelu przepływu gazu przez makropory. Dokonano numerycznego rozwiązania tej całki w kolejnych krokach czasu filtracyjnego drenażu metanu z pokładu węgla. Uzyskano stąd wyrażenie na wydatek desorbowanego gazu.

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