Supporting Information

Model for surface diffusion of adsorbed gas in nanopores of shale gas reservoirs

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Appendix A: Derivation of correction factor of apparent permeability of bulk gas in nanopores of shale gas reservoirs

Shale reservoirs are characterized by a myriad of nanopores. The shale reservoirs are theoretically considered to be the integration of capillaries and matrix as the nanopores are assumed to be the capillaries. In this paper, this assumption has been put forward for the calculation in the following section. The shale reservoir is represented by a cube with the porosity of φ , the permeability of k_a , the sectional area of A_b , the length of l_b and consisting of *n* nanopores. Consequently, it can be further achieved from the assumption that there exist *n* capillaries with an average permeability of k_{tt} , an average radius of r_t , an average length of l_t , and an average sectional area of A_t in the cube, i.e.; the shale reservoir.

The gas flux of the shale reservoir consisting of n capillaries can be written in the following equation without consideration of absorbed gas:

$$q_b = n \frac{k_{tt} A_t}{\mu} \frac{dp}{dl_t}$$
(A1)

In other ways, the gas flux can be also represented by

$$q_b = \frac{k_a A_b}{\mu} \frac{dp}{dl_b}$$
(A2)

Then the permeability k_a can be derived from the comparison of Eq. (A1) and Eq. (A2) as follows:

$$k_a = \frac{nA_tk_u}{A_b} \frac{dl_b}{dl_t}$$
(A3)

In the shale reservoir, the relationship between the capillary size and the capillary number can be expressed as

$$n = \frac{\phi A_b}{A_t} = \frac{\phi A_b}{\pi r_t^2} \tag{A4}$$

Moreover, the tortuosity of the nanopores can be written as

$$\tau = \frac{l_t}{l_b} \tag{A5}$$

where the tortuosity of the nanopores can be tested by the diffusion experiments.

Substituting Eq. (A4) and Eq. (A5) into Eq. (A3), we can get

$$k_a = \frac{\phi}{\tau} k_{tt} \tag{A6}$$

Then a correction factor of apparent permeability in the nanopores of the shale reservoir can be expressed as

$$\zeta_{mb} = \frac{\phi}{\tau} \tag{A7}$$

Eq. (A7) indicates that the porosity and tortuosity have pronounced influences on the gas transport efficiency.

Appendix B: Derivation of correction factor of surface diffusion of adsorbed gas in nanopore walls of shale gas reservoirs

The assumption made in **Appendix A** is also suitable here. Additionally, gas adsorption on nanopore walls of the shale reservoir is regarded as Langmuir monolayer adsorption and the height of the adsorption monolayer is set to be equivalent to the diameter of a gas molecule $d_{\rm M}$. Therefore, the bulk gas flowing sectional area $A_{\rm a}$ in the nanopores can be described as

$$A_a = \pi \left(r_t - d_M \right)^2 \tag{B1}$$

The adsorbed gas diffusion sectional area A_s in nanopores can be expressed as

$$A_s = \pi r_t^2 - \pi \left(r_t - d_M\right)^2 \tag{B2}$$

By a combination of Eq. (B1) and Eq. (B2), the ratio of A_s to A_a , A_{s-a} , can be achieved as

$$A_{s-a} = \frac{A_s}{A_a} = \left(1 - \frac{d_M}{r}\right)^{-2} - 1$$
(B3)

The bulk gas flux of nanopores can be written as follows:

$$q_b = A_a \frac{k_t}{\mu} \frac{dp}{dl_t} \tag{B4}$$

The surface diffusion flux in the walls of nanopores can be expressed as

$$q_s = A_s \frac{k_s}{\mu} \frac{dp}{dl_t}$$
(B5)

Eq. (B5) can be rearranged with consideration of Eq. (B3) as follows:

$$q_s = A_a \frac{A_{s-a}k_s}{\mu} \frac{dp}{dl_t}$$
(B6)

According to Eq. (B4) and Eq. (B6), the sum of the bulk gas flux and the surface diffusion flux in the nanopores wall can be derived:

$$q_{b-s} = q_b + q_s = A_a \frac{\left(k_{tt} + A_{s-a}k_s\right)}{\mu} \frac{dp}{dl_t}$$
 (B7)

By a combination of Eq. (A7), Eq. (B3) and Eq. (B7), the correction factor of gas diffusion in the nanopore walls of the shale reservoir, ζ_{ms} , can be expressed as

$$\zeta_{ms} = \zeta_{mb} A_{s-a} = \frac{\phi}{\tau} \left[\left(1 - \frac{d_M}{r} \right)^{-2} - 1 \right]$$
(B8)