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Mathematical model and numerical simulation of porous media gas-water fluid- solid coupling with considering gas adsorption

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Abstract
In order to understand the complex interaction between gas-water two-phase seepage and stress field with gas adsorption, a mathematical model of gas-water fluid-solid coupling for rock-coal porous media was established based on the stress equation, mass conservation equation, Darcy's law and gas adsorption mass equation. Using the COMSOL software with self-defined function codes, the simulation of seepage in rock-coal porous media with random-generated pore structures was carried out. The results indicate that the pressure of closed pores is larger than that of connected pores in saturated rock-coal porous media, and gas is difficult to get through the reservoir. As the pressure of pores increases, the volumetric strain increases, while the weighting of the adsorption strain decreases, appearing a weak influence on the matrix deformation in rock-coal. Under the present simulation conditions, the difference of magnitude between the volumetric strain and the adsorption strain is about 10^3, where the adsorption strain has a less influence on permeability, and permeability increases as volume strain increases, which conforms to exponent law.
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Keywords: Rock-coal porous media ; Two-phase flow; Flow-solid coupling; Adsorption.

1. Introduction

Fluid migration in rock-coal porous media can change the pore pressure, which will cause deformation of solid skeleton and lead to the changes of porosity and permeability, in return, the changes will influence fluid flow. The essence of above phenomenon is fluid-solid coupling process. Therefore, it is of great significance to study the gas-water two-phase fluid-solid coupling theory of porous media to provide a guidance to project practice.

In recent years, different studies about fluid-solid coupling theory for rock-coal porous media have been carried out. F.S. Karn et al. [1]studied the migration mechanism of gas in coal seam, the result showed that gas seepage and coal bed structure influenced each other, fluid-solid coupling theory was appropriate for the research of gas migration in coal seam. Later, Reucroft et al. [2] performed experimental research on adsorption strain of coal under 0.15MP pressure, the studies have shown that gas content in coal seam is negatively related to adsorption swelling deformation. In the theoretical research, Gorucu F B et al. [3] established the theoretical model of swelling strain caused by gas adsorption in coal from the perspective of thermodynamics, which proves that the influence of adsorption swelling force on gas migration in coal seam cannot be ignored. Cui et al. [4] established gas migration model considering diffusion, the model can accurately estimate the gas transmission characteristics in porous media and permeability and diffusion coefficient of porous media. Ramon G. Bentsen [5] established the coupling equation of air and water phase seepage flow in porous media on the basis of Kalaydjian's transport equation. Fanfan Sun et al. [6] found out that gas flow plays unimportant role on water transport form by simulating single-phase flow and gas-water phase flow. Schrefler B A et al. [7] developed a fully coupled model for water flow and airflow in deformable porous media, which is validated with respect to a documented experiment on saturated soil behavior.

In conclusion, previous studies have confirmed that skeleton deformation and fluid migration influence each other. However, there are few studies on the theory of gas-water two-phase fluid-solid coupling with considering the gas adsorption and diffusion effects. In this paper, on the basis of previous research, mathematical model of gas-water fluid- solid coupling is established considering porous media skeleton deformation caused by gas diffusion, adsorption strain and pore pressure. Using the COMSOL software with self-defined function codes, the simulation of seepage in rock-coal porous media with random-generated pore structures was carried out, in order to provide theoretical basis in engineering practice.

2. Theoretical modeling

A mathematic model was developed to describe the gas/-water two-phase rock-coal porous media seepage process. The mathematic model mainly includes the coupling of porous media deformation equation, seepage equation and gas adsorption equation in the process of rock-coal porous media seepage. In order to simplify the analysis, the following assumptions are made:

1. The relations between stress and strain in the deformation of skeleton particles are in accord with elastoplasticity constitutive model;
2. Gas phase exists in detached state and adsorption state;
3. Gas is in free state according to ideal gas state equation;
4. Water and gas seepage are in accordance with Darcy’s law;

2.1 Rock-coal porous media deformation equation

Fluid migration in rock-coal porous media can change the pore pressure. At the same time, the skeleton will occur deformation effected by effective stress when there is plus a load, and the stress of porous media is in the state of static equilibrium. Stress field equation is established based on effective stress theory, combining elastoplasticity geometry equation, constitutive equations and balance equation:

$$F_i - \alpha\nabla p - \left\{ 3G\nabla^2 u + \frac{G}{1-2\vartheta}\begin{bmatrix} (\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial x\partial y} + \frac{\partial^2 u}{\partial x\partial z}) + (\frac{\partial^2 \vartheta}{\partial x\partial y} + \\ \frac{\partial^2 \vartheta}{\partial y^2} + \frac{\partial^2 \vartheta}{\partial x\partial z}) + (\frac{\partial^2 w}{\partial x\partial z} + \frac{\partial^2 w}{\partial y\partial z} + \frac{\partial^2 w}{\partial z^2}) \end{bmatrix} \right\} = 0 \tag{1}$$

where σ is total stress, G is shear modulus, ϑ is poisson's ratio, Fi is Volume force, P is pore pressure.

2.2 Porosity and permeability equations

The permeability of porous media is influenced by skeleton deformation, pore structure and gas adsorption. The K-C formula [8] reflects the relationship between the permeability and porosity:

$$\mathrm{k} = \frac{\varphi}{k_z S_p^2} = \frac{\varphi^3}{k_z \sum^2} \tag{2}$$

where S_p is pore surface area of unit of pore volume, V_P is total pore volume, $\sum$ is pore surface area of unit volume of porous media.

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Because of the skeleton deformation of rock-coal porous media by the effect of adsorption of the pore surface, its porosity will change. Taking adsorption and skeletal deformation into consideration, the porosity equation can be derived:

$$\varphi = \frac{\varepsilon_v - \varepsilon_a + \varphi_0}{1 + \varepsilon_v} \tag{3}$$

where φ_0 is porosity, ε_v is volumetric strain, which is caused by the effective stress changes, the governing equation is expressed as:

$$\varepsilon_{\mathrm{v}} = \frac{\Delta V_h}{\Delta V_{ho}} \tag{4}$$

Y Zhou [9] found porosity has been changing with pressure and temperature. Based on the fact, simplified porosity equation can be obtained on the basis of this, that is:

$$\frac{\partial \varphi}{\partial t} = \alpha \frac{\partial \varepsilon_v}{\partial t} + \frac{1-\varphi}{k_s} * \frac{\partial p}{\partial t} \tag{5}$$

That the total surface area of particles of rock-coal porous media unit is approximately constant, thus the formula is given as:

$$\frac{k}{k_0} \approx \frac{\varphi V_P^2}{\varphi_0 V_{P0}^2} = \frac{1}{(1+\varepsilon_V)^3}(1 + \frac{\varepsilon_V - \varepsilon_a}{\varphi_0})^3 \tag{6}$$

Assuming that the volume strain $|\varepsilon_V| < 10\%$, $\frac{1}{(1+\varepsilon_V)^3} = \frac{1}{1+\varepsilon_V}$ and permeability equation is:

$$k = \frac{k_0}{1+\varepsilon_V}(1 + \frac{\varepsilon_V - \varepsilon_a}{\varphi_0})^3 \tag{7}$$

Wherein, adsorption deformation equation [10] is:

$$\varepsilon_a = \frac{a\rho RT}{EV_0}\ln(1+bp) \tag{8}$$

where a and b are adsorption constant, E is elastic modulus of porous media, R is constant, V_0 is initial pore volume.

2.3 Gas flow in rock-coal porous media coupled equation

Gas exists in the rock-coal porous media including adsorption and free state; gas adsorption follows Langmuir equation; Free gas follows ideal gas state equation; gas diffusions follows Fick's law; gas seepage is in accordance with Darcy's law. So gas flow in rock-coal porous media coupled equation is given as:

$$\rho\alpha \frac{\partial \varepsilon_v}{\partial t} + (\varphi + p\frac{1-\varphi}{k_s} + \frac{abp_a\rho_s}{(1+bp)^2})\frac{\partial p}{\partial t} + \nabla\left[-\frac{k}{u}p\nabla p - Dabp_a\rho_s\frac{p}{1+bp}\right] = 0 \tag{9}$$

where D is diffusion coefficient, u is velocity component, ρ_s is gas density.

2.4 Gas, water two-phase rock-coal porous media seepage coupling equation

Gas and water seepage is in accordance with Darcy's law, and each fluid phase follows this principle correspondingly:

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$$\varepsilon_a \rho_L \frac{\partial s\varphi}{\partial t} - \nabla(\rho_L \frac{\mathrm{k}k_{r,L}}{u_L}) = 0 \tag{10}$$

$$\frac{\partial\left[\varphi\rho_g(1-s)\right]}{\partial t} - \nabla(\rho_g \frac{\mathrm{k}k_{r,g}}{u_g}) = 0 \tag{11}$$

Water and gas two-phase relative permeability equations are:

$$k_{r,L} = S^L \left[1-(1-S^{\frac{1}{m}})^m\right]^2 \tag{12}$$

$$k_{r,g} = (1-S)^L (1-S\frac{1}{m})^{2m} \tag{13}$$

where L is Van Genuchten parameter, $kr,_L$ is water phase relative permeability, kr,g represents gas relative permeability.

Pore pressure concludes gas phase pressure and water pressure. Then the gas phrase and water phase's total pressure can be calculated according to the following formula:

$$p = sp_L + (1-s)p_g \tag{14}$$

The effective saturation [11] equation is:

$$s = \left[1+\left|\frac{\alpha(p_g - p_L)}{\rho_L g}\right|^n\right]^{-m} \tag{15}$$

Considering the effective saturation, the mass equation of the gas in the pore is:

$$m_g = \frac{abp_g}{1+bp_g}\rho_{ga}\rho_s + \beta p_g \varphi(1-s) \tag{16}$$

Introducing the formula (13), (14), (16) into equation(11) gas seepage coupling equation can be obtained:

$$\begin{aligned}&\beta\varphi s\frac{\partial p_g}{\partial t} + (1-s)\beta p_g \alpha \frac{\partial \varepsilon_v}{\partial t} + (1-s)\beta p_g \frac{1-\varphi}{k_s}(\frac{\partial s}{\partial t}(p_L - p_g) + s\frac{\partial pL}{\partial t} + (1-s)\frac{\partial p_g}{\partial t})\\ &-\beta p_g \varphi \frac{\partial s}{\partial t} + \frac{abp_{ga}\rho_s}{(1+bp)^2}\frac{\partial p_g}{\partial t}\nabla\left[-\beta p_g \frac{kk_{rg}}{u_g}\nabla p_g - D\nabla(\frac{abp_g\rho_{ga}\rho_s}{(1+bp_g)})\right] = 0\end{aligned} \tag{17}$$

Similarly, Introducing the formula (12), (14),(15) into equation (10) water seepage coupling equation can be obtained:

$$\left(\varphi + s\frac{1-\varphi}{k_s}(\rho_L - \rho_g)\right)\frac{\partial s}{\partial t} + s\left(\alpha\frac{\partial \varepsilon_v}{\partial p_L}\frac{1-\varphi}{k_s}(s+(1-s)\frac{\partial p_g}{\partial p_L}\right)\frac{\partial p_L}{\partial t} + \nabla(-\frac{kk_{r,L}}{u_L}\nabla P_L) = 0 \tag{18}$$

3. Numerical simulation

3.1 Geometric model building

The simulation of gas and water seepage in rock-coal porous media containing saturated water with random-generated pore structures was carried out. By using the random generation-growth method which is put forward by Moran Wang [12], who had taken actually observed on rock-coal porous media and obtained the statistics of its structure. And combined with computer technology, the bitmap format stochastic model of porous media is gotton, as shown in Figure 1; The main property parameters of model as shown in Table 1.

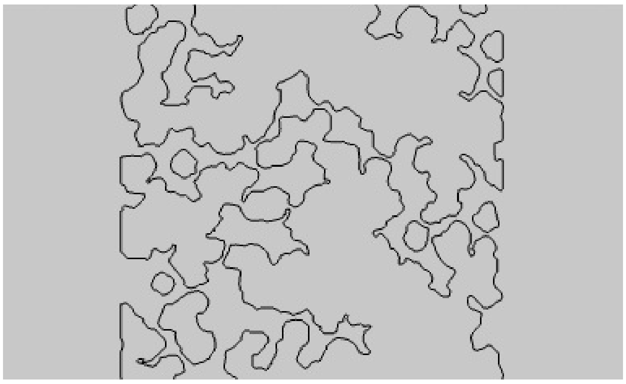

Figure 1. Geometric model.

Table 1. The main property parameters.

Water Density (kg/m³)	1000	adsorption constant [1/MPa]	1.211
Hydrodynamic viscosity [Pa*s]	1e-3	Elastic modulus of rock-coal[MPa]	3000
The gas dynamic viscosity [Pa*s]	1.84e-5	The initial porosity	0.3
Diffusion coefficient [m²/d]	2.1e-3	Initial solid density [g/cm³]	1.35
The temperature[K]	300	The initial permeability[m²]	8.8e-13
Gas molecular [g/mol]	16	Initial gas density [g/cm³]	0.717
adsorption constant [cm³/g]	20	Poisson's ratio	0.33

3.2 Control equation and the definite condition

The simplified water phase and gas phase control equation in the process of gas-water two-phase rock-coal porous media seepage are respectively as follows:

$$\left\{ \begin{array}{l} \left(\rho_L\phi+\rho_L S\frac{1-\phi}{K_s}\left(P_L-P_g\right)\right)\left[(-\mathrm{mn})\left[1+\left|\frac{\alpha_f(P_g-P_L)}{\rho_L g}\right|^n\right]^{-m-1}\left(\left|\frac{\alpha_f(P_g-P_L)}{\rho_L g}\right|^{n-1}\left(\frac{\alpha_f(\frac{\partial P_g}{\partial P_L}-1)}{\rho_L g}\right)\right)\right] \\ +\rho_L S\left(\alpha\frac{\partial\varepsilon}{\partial P_L}+\frac{1-\phi}{K_s}\left(S+(1-S)\frac{\partial P_g}{\partial P_L}\right)\right) \end{array}\right\}\frac{\partial P_L}{\partial \mathrm{t}}$$

$$+\nabla\left(-\rho_L S\frac{kk_{rl}}{u_L}\nabla P_L\right)=0 \tag{19}$$

The initial conditions:

$$\begin{array}{l} p_L(t_0)=C \\ p_g(t_0)=C \end{array} \tag{20}$$

The initial conditions for solid mechanics: the initial displacement and velocity of stress field are zero.
The flow boundary conditions: Upper and lower boundaries are impermeability:

$$\frac{\partial P}{\partial X}=0, \mathrm{y}=\pm 4.7\,\mathrm{cm},\ p_L=C, p_g=C; X=\pm 10\,\mathrm{cm} \tag{21}$$

Solid mechanics boundaries (left and right) are displacement constraints.

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3.3 Model validation

The relationship between the relative permeability and saturation of the gas-water phase is shown in Figure 2. It can be found that the gas relative permeability (Krg) decreases with the increasing water saturation, meanwhile, the water relative permeability (Krw) increases. Besides, two phase curves increases at the saturation of 0.6 and Krg is higher than Krw when the saturation is lower than 0.6. Moreover, the decreasing rate of Krg gradually slows down as saturation increases. However, the increasing speed of Krw grows quickly. The simulation results are closed to the previous experimental results [13], which proves the model is reliable.

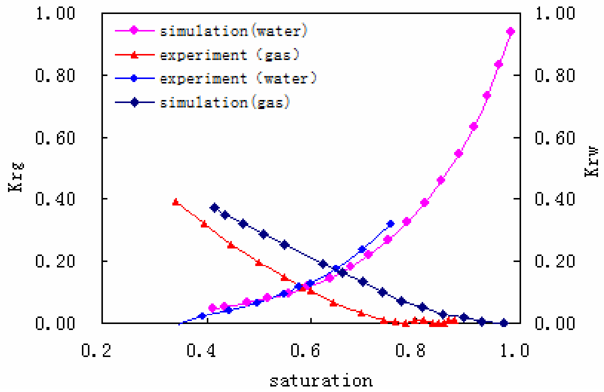

Figure 2. Relative permeability curves.

4. Results and discussion

4.1 Pressure variation

Figure 3 and Figure 4 are gas phase and water phase pressure contours distribution at different moments. It can be seen that the pressure decreases gradually along the flow direction from the inlet, and the loss of pressure increases with the increasing fluid percolation. When the gas and water pass through simultaneously, the gas content in gas-water mixture increases gradually, the conductivity decreases, and the pressure of the whole fluid region increases gradually [14]. At the same time, the gas pressure is smaller than that of water, which is proved water is much easier to pass forward. The pore structure of rock-coal porous media is complex, and the gas will preferentially select the large pore channel to seepage. The water-tightness is enhanced due to the capillary pressure in the narrow pore channels, and with considering the gas adsorption, so the gas is relatively difficult to pass through the coal-rock containing saturated water, which will reduce the gas extraction efficiency.

Figure 5 is the variation of the closed pore and connected pore gas pressure graph. The initial state fluid pressure is about 0.1MPa, the inlet pressure is 0.3MPa. It can be seen that the change trend of the pressure at the closed porosity is almost the same as that of the connected gap, which increases with time and then reaches the steady state. At steady state, the pore pressure is 0.3 MPa, which is the same with the inlet pressure, which is higher than that of the connected pore (0.18 MPa), but its stabilization time is lagging behind. Gas in the closed pores is relatively easy to gather into the gas state, the pressure is large; Gas in the closed pores is relatively easy to gather into aggregation state, the pressure is relatively large. The gas pressure in connected pore is relatively small, and the pressure in the flow field is lower than 1.13MPa, which is lower than the gas outburst safety pressure [15]. The results indicate that controlling the inlet pressure of rock-coal is one of the effective measures to reduce gas outburst accident.

4.2 Volumetric strain and adsorption strain

Figures 6 and 7 show the volume strain and adsorption strain distribution under low and high pressure. It can be seen that the volumetric strain and the adsorption strain of coal are increasing with the increasing inlet pressure, and the deformation area is mainly concentrated in the main pore channel. The deformation of framework is anisotropic due to the inhomogeneous distribution of pore structure. The maximum adsorption strain increases from 1.14×10^{-6} to 1.62×10^{-5} when the condition changes from low pressure to high pressure. Increases to the original 14.21 times, which is in a good agreement with the results of Levinel's [16]. The maximum volume strain of low pressure increases 1.65×10^{-4} to 4.6×10^{-3}.

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Increases to the original 7.8 times. Under the condition of same booster (0.3MPa-1.8MPa), adsorption train increment is greater than that of volume strain.

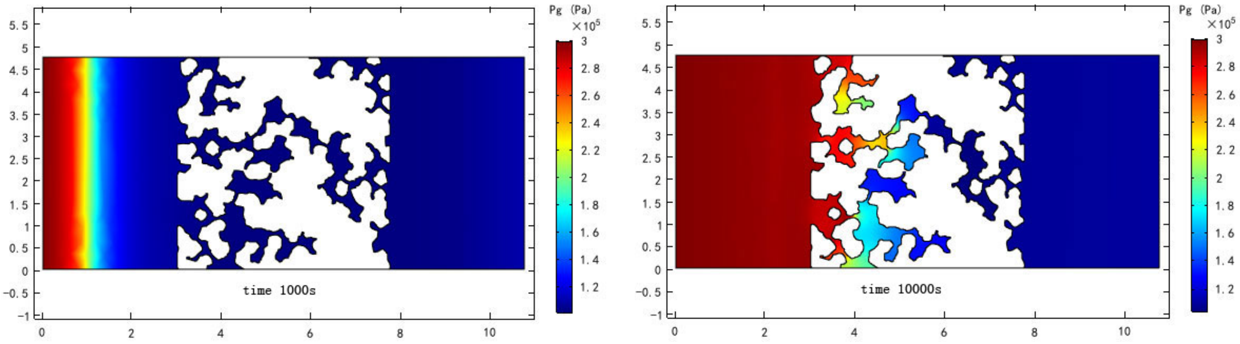

Figure 3. Gas phase pressure contours.

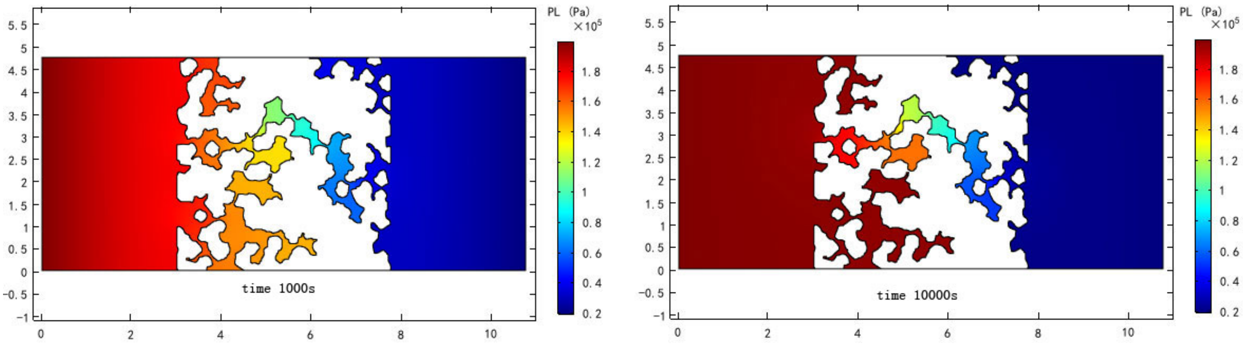

Figure 4. Water phase pressure contours.

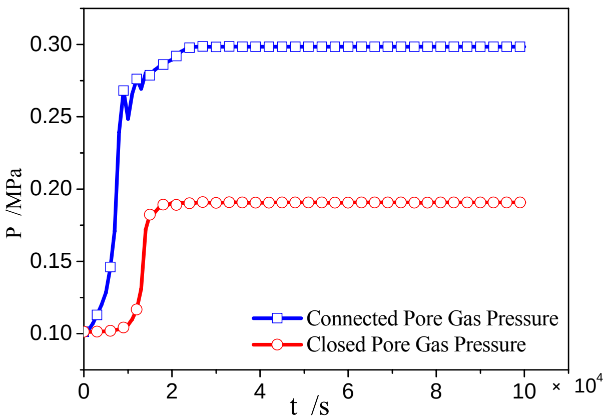

Figure 5.Variation of the closed pore and connected pore gas pressure.

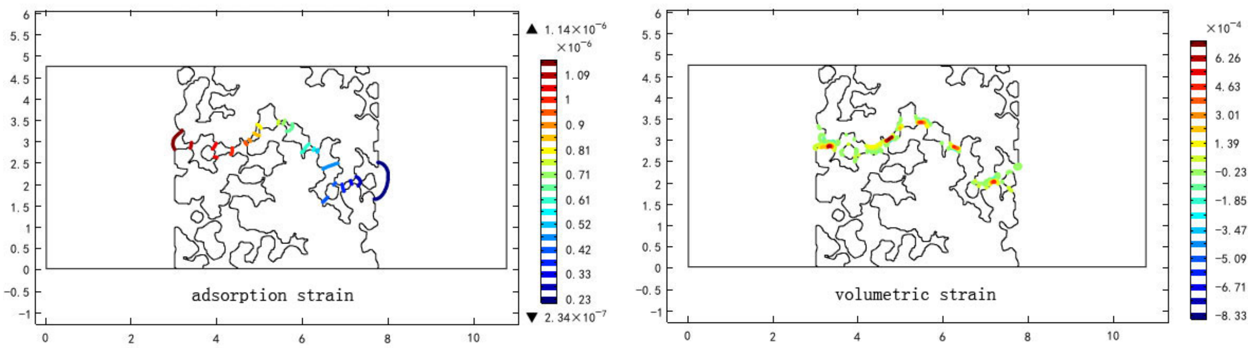

Figure 6. Volumetric strain and Adsorption strain under low pressure.

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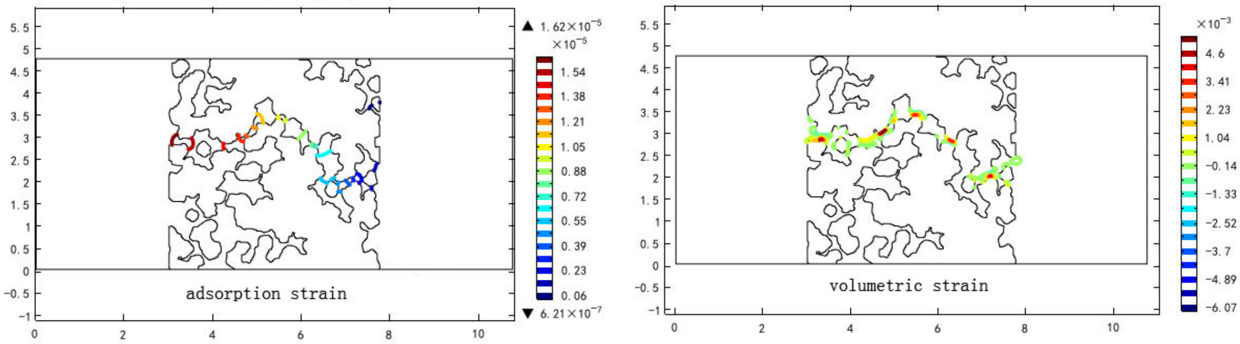

Figure 7. Volumetric strain and Adsorption strain under high pressure.

Figure 8 shows the simulated results of adsorption strain and volumetric strain changes with increasing pressure. In the process of gas flowing through rock-coal porous media, considering adsorption effect, pore pressure will change that causing adsorption strain. Adsorption strain will produce adsorption stress that has an impact on the effective stress, causes the deformation of skeleton particles, which results in volumetric strain. Volumetric strain is affected by both pore pressure and effective stress with considering adsorption. It can be seen that adsorption strain and volumetric strain are proportional to permeability. The rate of increase of adsorption strain gradually slowed down, showing a non-linear trend, which is consistent with Harpalani [17] experimental conclusion. Volumetric strain increases exponentially which is in a good agreement with the results of M. Vandamme [18]. Under the same pressure, the magnitudes of the differences between volume deformation and adsorption deformation are 10^3. Thus, the volumetric strain increases with the increasing pore pressure, wherein the weighting of strain adsorption is smaller, which has a less influence on the deformation of the skeleton in porous media.

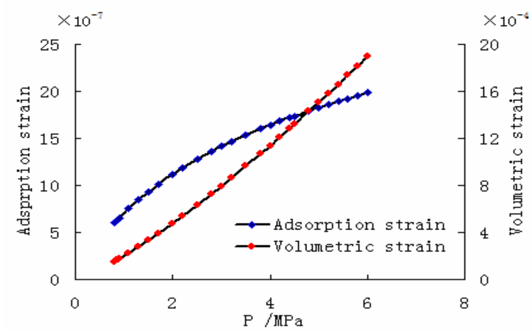

Figure 8. Variation of adsorption strain and volumetric strain.

4.3 Permeability variation

Figure 9 shows permeability curves under low pressure and high pressure. It can be seen permeability variation is small relative to the initial permeability of 8.8×10^{-13}m2.Considering the conditions of gas phase pressure is 0.3 MPa at the entrance, which can be found that the change of permeability is very small according to the permeability change equation (7). When the inlet pressure is 1.8MPa, the maximum permeability reaches $9.1\times10^{-13}m^2$, and the permeability changes greatly. The effective connectivity of the pores reduces which is caused by gas adsorption of the pore surface, and permeability decreases. The permeability increases with the increasing volume strain, which is due to the shrinkage of porous matrix particles with the increase of pore pressure, resulting in the increase of the effective connectivity area.

Figure 10 shows the variation of permeability with increasing pressure. It can be seen that permeability increases with increasing pressure. Adsorption strain is inversely proportional to permeability, and volumetric strain is proportional to permeability. The magnitude of adsorption strain is so smaller relative to the volumetric strain that it has a less effect on permeability. So permeability changing trend is the same as volumetric strain, indicating that the permeability change is less affected by adsorption strain, which is consistent with the previous conclusions, and proves that the simulated results which are presented herein have certain reliability.

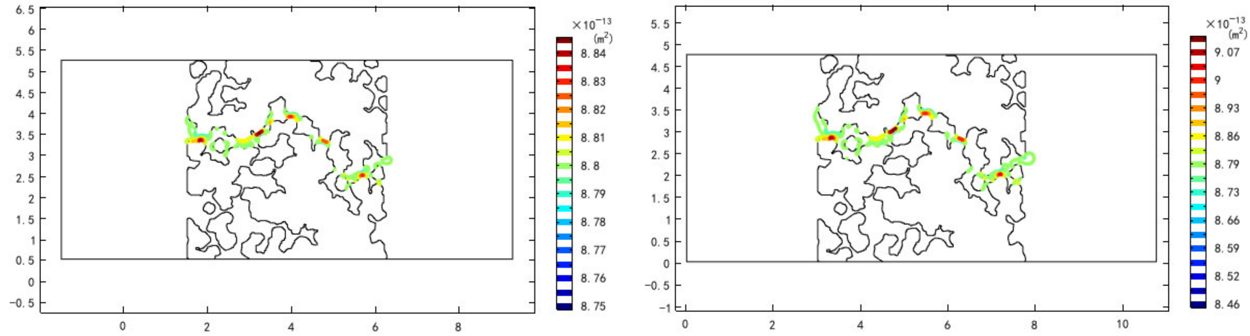

Figure 9. Permeability contour maps under low pressure and high pressure.

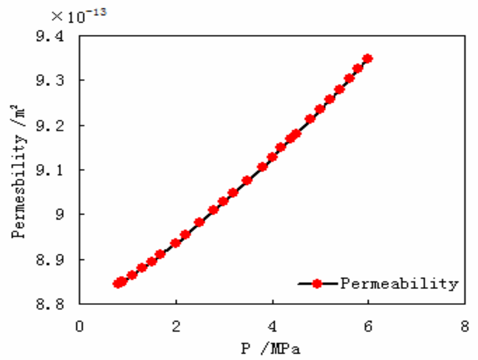

Figure 10. Variation of permeability.

5. Conclusion

1. The mathematical model of fluid-solid coupling of gas phase is established with considering gas absorption, stress equation. Combined with two-phase Darcy's law, saturation equation, relative permeability equation, mathematical model of gas-water two-phase fluid-solid coupling for rock-coal porous media is established based on the model of gas phase.
2. Using the COMSOL software with self-defined function codes, the simulation of seepage in rock-coal porous media with random-generated pore structures was carried out. The results indicate that the pressure of closed pores is larger than that of connected pores in saturated rock-coal, and the diffusion rate of gas phase is larger than that of water phase, and gas is difficult to get through the reservoir. As the pressure of pores increases, the volumetric strain increases, while the weighting of the adsorption strain decreases, appearing a weak influence on the matrix deformation in rock-coal.
3. Under the present simulation conditions, by analyzing the relationship among permeability, volumetric strain, and adsorption strain under various pressure conditions, the result indicates that the difference of magnitude between the volumetric strain and the adsorption strain is about 10^3, where the adsorption strain has a less influence on permeability, and permeability increases as volume strain increases, which conforms to exponent law.

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