Diffusion of Gases in Porous Environments, Taking into Account the Convective Component

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In this work we study the process of replacing gas in porous media considering convective motion of one of the gases and dependence of diffusion coefficients on the pressure in them. We have given the formulas to calculate the diffusion coefficients, which depend on the coefficients of interdiffusion of gases and pressure. The numerical experiment shows that the convective component has a significant impact on the process of mixing gases. **Key words:** gas replacing, porous media, diffusion convective component

There are little papers dedicated to the investigation of a multi-component gas in porous environment, which is primarily explained by the specificity and complexity of the tasks. Modeling these processes usually leads to the need for solving the nonlinear differential equations in partial derivatives or their systems with variable, in particular discontinuous, ratios under conditions of substantial uncertainty. The movement of a two-component gas mixed in a porous environment is a typical convection-diffusion process. During the gas movement in a porous process the convective component is an order higher than the diffuse one. Upon small convective velocity and in view of the gas mixing process the process of convection-diffusion must be considered simultaneously.

The diffusion of two gases without convective component is explained by the differential equation

$$\frac{\partial c}{\partial \tau}=\frac{\partial}{\partial x}\left(D\frac{\partial c}{\partial x}\right)+\frac{\partial}{\partial y}\left(D\frac{\partial c}{\partial y}\right)+\frac{\partial}{\partial z}\left(D\frac{\partial c}{\partial z}\right), \quad (1)$$

for given boundary conditions, where the D parameter means the coefficient of mutual diffusion of A and B gases. Many formulas are developed for its determination, including [1]

$$D_{AB}=\frac{T^{1,5}}{p(\sigma_A+\sigma_B)^2}\left(\frac{1}{m_A}+\frac{1}{m_B}\right)^{0,5},$$

where p, T is the pressure and temperature in the system, m_A and m_B – are the gas masses, s_A and s_B are the parameters of the Lennard-Jones potential.

Indian mathematicians, Saxena M. and Saxena S. proposed the following modified formula of Sazerland for the computation of the mutual diffusion of D_{AB} gases (c m ^{2}/ c) [1]:

$$D_{AB}=\frac{AT^{1,5}\left(\frac{1}{m_A}+\frac{1}{m_B}\right)^{0,5}}{p(V_A^{1/3}+V_B^{1/3})[1+(BT_{AB}/T)]},$$

where VA, VB, TA and TB are the critical volumes (cm^3/mol) and temperature (K) of gases, p is the pressure in atmospheres, $T_{A,B}=(T_A\ T_B)^{0,5}$. For nonpolar gases A=0.022023 and B=1.1756, while for systems consisting of a combination of polar and nonpolar gases A=0.022023 and B=1.90116. If the self-diffusion coefficients of D_{AA} and D_{BB} gases are known, *t*hen

$$D_{AB}=\sqrt{\frac{m_A+m_B}{2\sqrt{m_A m_B}}}\sqrt{D_{AA}D_{BB}}\ .$$

Let's consider a cylindrical source of gas injection, uniformly distributed along the axis. The area of the PSG reservoir is modeled with a cylinder divided by cylindrical surfaces into appropriate sub-areas filled with different gases and their mixture (Fig. 1): zone I is filled with the extracted gas, zone II occurs as a result of the displacement of the existing gas with a pumped gas, resulting in the jamming of a part of the pores, and area III is filled with injected gas. Then the equation for determination of the distribution of gas pressure in each subzone will look as follows [2,3]

$$\frac{\partial^2 p}{\partial r^2}+\frac{1}{r}\frac{\partial p}{\partial r}=\frac{\tilde{D}}{p_0}\frac{\partial p}{\partial \tau}\ , \qquad (2)$$

where r is the radius vector drawn from the well center according to Leybenzon:

with υ = 0.002 m/s

$$\tau=\frac{p_2}{p_0}t+\left(1-\frac{p_2}{p_0}\right)\frac{1-e^{-\beta t}}{\beta}\ ,\ D=\frac{m\mu}{k}\ ,\ \beta=\frac{p_0 k\lambda_m^2}{2m\mu}\ .$$

Here p_0 and p_2 are the initial value of the pressure and the pressure at the area boundary respectively. The solution of equation (2) with constant boundary conditions is given in [2-4].

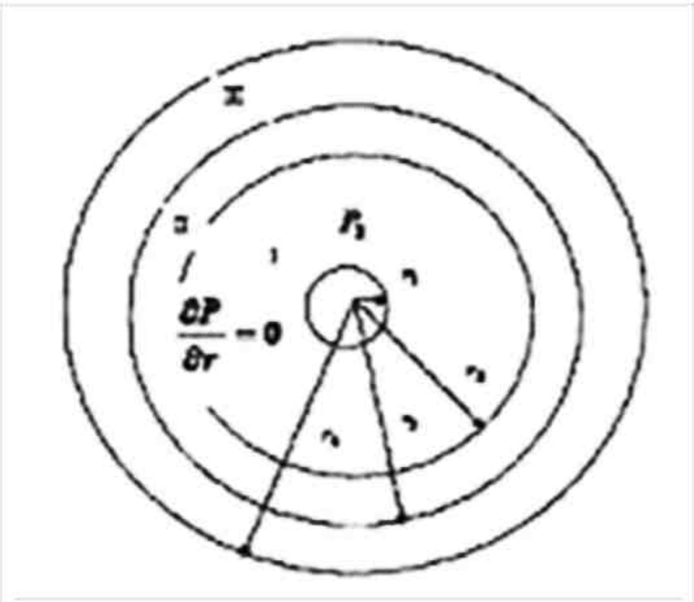

Fig. 1. PSG layer area distribution

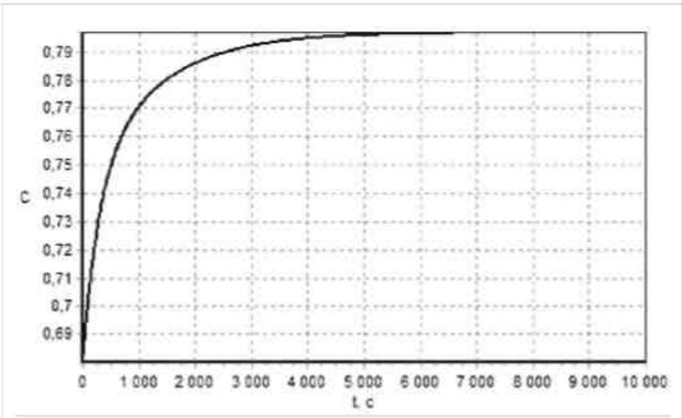

Fig. 2. The dependence of the diffusion coefficient c_z from time *t* at the distance of *r*= 32 m

If the pressure distribution is known, the velocity of the gas movement is determined as follows:

$$\upsilon = -\frac{\ }{\mu}\frac{\partial p}{\partial r}\ , \qquad (3)$$

Here μ is the absolute viscosity of gas, and *k* is the permeability of the layer occupied with gas. Equation (1) takes place in the second zone only if its boundary is not shifted. Otherwise, you must consider the velocity of the boundary movement. During the displacement of one gas with another the diffusion process should be considered, taking into account the convective component, i.e. the velocity of the first zone movement. Then the problem is reduced to solution of the diffusion equation with the convective component

$$\frac{\partial c}{\partial \tau} + \upsilon\frac{\partial c}{\partial r} = D\left(\frac{\partial^2 c}{\partial r^2} + \frac{1}{r}\frac{\partial c}{\partial r}\right),$$

under appropriate boundary conditions. Here υ is the velocity of the gas in the first zone determined with formula (3). For numerical analysis of the influence of the convective component on the diffusion process a simpler model is considered, namely the gas diffusion in the layer with *l* thickness, described by the equation

$$\frac{\partial c}{\partial \tau} + \upsilon\frac{\partial c}{\partial r} = D\frac{\partial^2 c}{\partial r^2}\ , \qquad (4)$$

under appropriate boundary conditions recorded as $c_1(r) = c(r, 0)$, $c_2(r) = c(r,l)$ $c_3(t) = c(0, t)$.

For consistency of conditions it is required to satisfy the equality of $c_1(0) = c_3(0)$.

Solution of equation (4) will be searched using the Laplace transformation. For constant coefficients equation (4) will look as follows:

$$\bar{c}'' - b\bar{c}' - p_1\bar{c} = -c_{11}\ , \qquad (5)$$

Here b= Y /*D*, p_1= S /*D*, $c_{11} = c(r, 0)\ /D$. We assume that the *b* and p_1 parameters are constant. The general solution of a homogeneous equation will look as follows:

$$\bar{c}_z = A_e^{\lambda_1 r} + Be^{-\lambda_2 r},$$

where

$$\lambda_1 = \lambda_{11} - \lambda_{12}, \ \lambda_1 = \lambda_{11} + \lambda_{12}, \ \lambda_{11} = \frac{\upsilon}{2D}, \ \lambda_{12} = \frac{1}{2}\sqrt{\left(\frac{\upsilon}{D}\right)^2 + \frac{4s}{D}}.$$

A partial solution of the differential equation (5) depends on its right side, in particular, the method of constants variation leads to relation:

$$\bar{c}_{ch} = \frac{1}{\lambda_2 - \lambda_1}\left(e^{\lambda_1 r}\int c_{11} e^{-\lambda_1 y} dy + e^{-\lambda_2 r}\int c_{11} e^{-\lambda_2 y} dy\right).$$

If *c11* function is identically constant, then the partial solution will be ***cch = - cn / XlX2.*** At sustainable boundary conditions the general solution of the problem will be as follows

$$\bar{c}_z = -\frac{c_{11}}{\lambda_1\lambda_2} + c_{31} e^{\lambda_{11} r}\frac{sh\lambda_{12}(l-r)}{sh\lambda_{12} l} + c_{21} e^{\lambda_{11}(l-r)}\frac{sh\lambda_{12} r}{sh\lambda_{12} l}.$$

The last equality it is marked as

$$c_{31} = \bar{c}(0,s) + \frac{c_{11}}{\lambda_1\lambda_2}, \ c_{21} = \bar{c}(l,s) + \frac{c_{11}}{\lambda_1\lambda_2}.$$

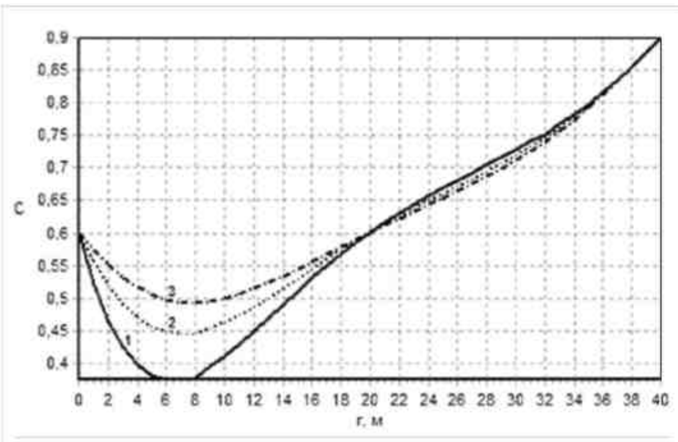

Fig. 3. The dependence of the diffusion coefficient c_z on distance for time t = 400s and different values of the convective velocity υ ={0.004; 0.003; 0.002} m/s, where curve 1 represents the velocity of υ = 0.004 m/s, curve 2 υ = 0.003 m/s, and curve 3 υ = 0.002 m/s

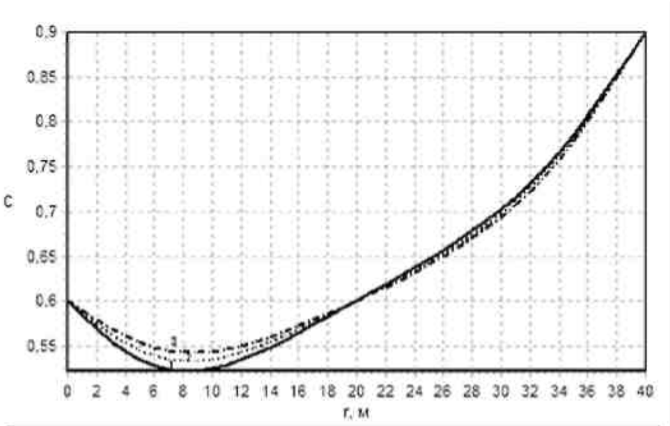

Fig. 4. The dependence of the diffusion coefficient c_z on distance for time t= 400s and different values of the convective velocity υ = {0.001; 0.0005; 0} m/s, where curve 1 represents the velocity of υ = 0.001 m/s, curve 2 υ = 0.0005 m/s, and curve 3 υ = 0 m/s

The general solution in Laplace images is as follows:

$$\bar{c}_z = \frac{c_1}{s} + (c_3 - c_1)\frac{1}{s}e^{\lambda_{11}r}\frac{sh\lambda_{12}(l-r)}{sh\lambda_{12}l} + (c_2 - c_1)\frac{1}{s}e^{\lambda_{11}(l-r)}\frac{sh\lambda_{12}r}{sh\lambda_{12}l}.$$

Let's mark

$$\Phi(a,b,s) = \frac{1}{s}\frac{shaq}{shbq}.$$

Then

$$\bar{c}_z = \frac{c_1}{s} + (c_3 - c_1)e^{\lambda_{11}r}\Phi(l-r,l,s) + (c_2 - c_1)e^{\lambda_{11}(l-r)}\Phi(r,l,s).$$

$$\Phi(a,b,s) = \frac{1}{s}\frac{shaq}{shbq} = \frac{a}{b} + \frac{2}{\pi}\sum_{k=1}^{\infty}\frac{(-1)^k}{k}\sin\frac{k\pi a}{b}\frac{q^2}{q^2 + \left(\frac{k\pi}{b}\right)^2}.$$

The original image F(a, b, c) will be sought by its decomposition into simple fractions

Whereas

$$q^2 = s + \frac{\upsilon^2}{4D},\ b = l/\sqrt{D},\ a = \left\{(l-r)/\sqrt{D},\ r/\sqrt{D}\right\},$$
$$a/b = \{(l-r)/l,\ r/l\},$$

$$\frac{1}{s}\frac{q^2}{q^2 + (k\pi/b)^2} = \frac{1}{s}\frac{s + \lambda_{13}^2}{s + \lambda_k^2}$$

then the original image is

$$\lambda_{lr}^2=\lambda_{13}^2+(k\pi/b)^2,\ \lambda_{13}=\upsilon/2\sqrt{D},$$

where

$$e^{-\lambda_{lr}^2 t}+\lambda_{13}^2\frac{1-e^{-\lambda_{lr}^2 t}}{\lambda_{lr}^2}=e^{-\lambda_{lr}^2 t}+\frac{\lambda_{13}^2}{\lambda_{lr}^2}\left(1-e^{-\lambda_{lr}^2 t}\right).$$

is a function.

Then

$$\varphi(a,b,t)=\frac{a}{b}+\frac{2}{\pi}\sum_{k=1}^{\infty}\frac{(-1)^k}{k}\sin\frac{k\pi a}{b}\left(e^{-\lambda_{lr}^2 t}+\frac{\lambda_{13}^2}{\lambda_{lr}^2}(1-e^{-\lambda_{lr}^2 t})\right),$$

and finally

$$c_z=c_1+(c_3-c_1)e^{\lambda_{11}r}\varphi(l-r,l,t)+(c_2-c_1)e^{\lambda_{11}(l-r)}\varphi(r,l,t).$$

If the convective component is absent, i.e. $\upsilon = 0$, then $\lambda_{11}=\lambda_{13}=0,\ \lambda_{lr}^2=(k\pi/b)^2$,

and

$$\varphi_0(a,b,t)=\frac{a}{b}+\frac{2}{\pi}\sum_{k=1}^{\infty}\frac{(-1)^k}{k}e^{-\lambda_{lr}^2 t}\sin\frac{k\pi a}{b},$$

and

$$c_{z0}=c_1+(c_3-c_1)\varphi_0(l-r,l,t)+(c_2-c_1)\varphi_0(r,l,t).$$

From these solutions it is easy to get component Δs, which is describes the effect of convective motion on the diffusion coefficient:

$$\Delta c=c_z-c_{z0}=(c_3-c_1)\left[e^{\lambda_{11}r}\varphi(l-r,l,t)-\varphi_0(l-r,l,t)\right]+$$
$$+(c_2-c_1)\left[e^{\lambda_{11}(l-r)}\varphi(r,l,t)-\varphi_0(r,l,t)\right].$$

Table 1

The value of the diffusion coefficient for different values of the time *t* and coordinate *r* with $\upsilon = 0.002$ m/s and *T*= 10,000 K

t/r	0	8	16	24	32	40
0	0.6	0.3728	0.5591	0.6508	0.6800	0.9
2500		0.5582	0.6136	0.6966	0.7897	

5000		0.5688	0.6280	0.7087	0.7960	
7500		0.5702	0.6299	0.7103	0.7968	
10000		0.5704	0.6302	0.7105	0.7969	

Table 2

The value of the diffusion coefficient for different values of the time *t* and coordinate *r* with $\upsilon = 0.005$ m/s and T=400 K

t/r	0	8	16	24	32	40
0	0.5	0.3429	0.4466	0.5288	0.5906	0.9
100		0.4211	0.4618	0.5440	0.6663	
200		0.4559	0.4781	0.5601	0.7000	
300		0.4762	0.4987	0.5804	0.7196	
400		0.4909	0.5185	0.6001	0.7338	

The results were verified t during the computational experiments for different values of the input parameters. The convective gas movement velocity in underground storage reservoir was calculated by the formula (3), and the diffusion coefficient was determined as shown by the above formulas. The results of calculations are presented in tables and fig. (2-4) for the following values of the parameters l=40 m, D=0.05 (cm^2/s), $c(r, 0) = 0.06$, $c(0, t) = 0.6$, $c(l,t)$ = 0 9.

The results shown in Fig. 5 and 6 correspond to the following values of parameters l=32 m, D= 0.05 (cm^2/s) $c(r, 0) = 0.9$, $c(0, t) = 0.9$, $c(l,t) = 0$.

The analysis of the results shows that the convective component has a significant impact on the gas diffusion process. Despite the fact that the gas flow velocity in porous environments is small, its growth results in increased concentration of admixture.

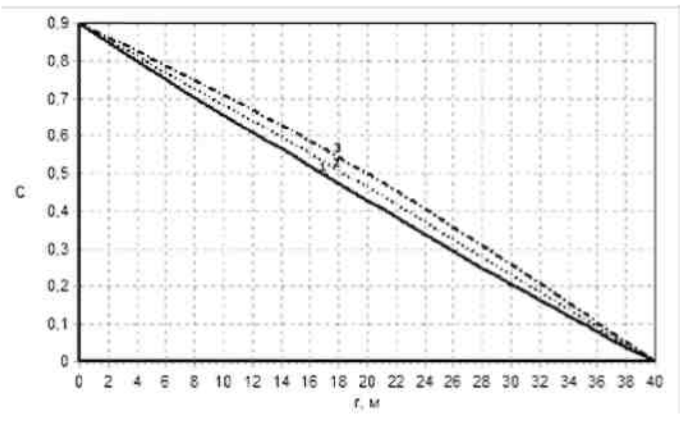

Fig. 6. Dependence of the diffusion coefficient c_z on distance for time t= 400s and different values of the convective velocity υ = {0.004; 0.002; 0} m/s, where curve 1 represents the velocity of υ = 0.004 m/s, curve 2 υ = 0.002 m/s, curve 3 υ = 0 m/s

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