
MODELLING OF INTERNAL TRANSFORMATIONS OF GAS PHASE IN POROUS MEDIA

 Geylani Panahov¹,  Eldar Abbasov¹,  Azer Ehmedov²,  Ibrahim Mamedov^{1*}

¹Institute of Mathematics and Mechanics, Baku, Azerbaijan

²Baku Engineering University, Baku, Azerbaijan

Abstract. The paper presents the research of temperature change in the investigated medium during dynamic expansion of gas (CO₂) generated in reservoir conditions, diffusion of carbon dioxide into the displacing fluid and their influence on the displacement process. In-situ gas generation can provide a way to control the non-equilibrium fractal state at the interface under displacement in a porous medium. The change from fractal growth to non-fractal growth can be characterised as a function of density and viscosity ratios. This effect is shown in the increase of hydrocarbon displacement coefficient due to the equalisation of densities of displacing and displaced agents as a consequence of the increase in gas saturation of the fluid.

Keywords: in-situ generation, carbon dioxide, diffusion, fractals, viscosity, density.

AMS Subject Classification: 35Q49, 74N25.

Corresponding author: Ibrahim Mamedov, Institute of Mathematics and Mechanics, B. Vagabzade 9, Baku, Azerbaijan, Tel.: +994515772877, e-mail: imamedoff1997@list.ru

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1 Introduction

Fluid filtration in porous media regarding the problems of flow of gas-liquid mixtures (reservoir fluids - oil, gas, water) in porous media is one of the actual problems of fluid mechanics. Research in the field of hydrocarbon displacement is of particular relevance in oil and gas production processes under conditions of reservoir pressure drop. These issues are mainly related to water and gas flow processes under injection in porous media and are aimed to solve the problem of oil displacement and reservoir pressure maintenance. A number of factors determined by viscous heterogeneity of displaced and displacing fluids during water injection into the reservoir, as well as formation heterogeneity in permeability, zonal heterogeneity of the reservoir accelerate water breakthrough to production wells. In this regard, there is a need to use other, more effective tertiary methods of impact on the reservoir system reviewed in Dake (1998), Muggeridge et al. (2014). Some examples of such methods are physical methods, thermal methods, gas injection (air, nitrogen, CO₂), water-gas mixtures, etc. noted in Assef & Pereira (2019), Bila et al. (2020), Speight (2019). Aqueous solutions of various chemical agents are also used at the final stages of oil field development to increase the displacement efficiency during waterflooding and to recover residual oil reserves from stagnant reservoir zones. Currently, the technology of enhanced oil recovery by using carbon dioxide as a displacing agent is one of the most effective and is aimed

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at the recovery of hard-to-recover oil reserves, as it noted in Bakhtiyarov et al. (2006); Ferer & Smith (1994); Mandrik et al. (2010); Gasimov et al. (2019). The distribution of injected CO₂ gas in oil saturated porous media is crucial for risk assessment and prediction of carbon dioxide application. This paper investigates the main characteristics of the process based on a kinetic diffusion approach to the phenomena under consideration. This involves studying the temperature change in dynamic expansion of in-situ generated gas (CO₂), diffusion of carbon dioxide into the displacing fluid and its effect on the displacement process, results of which presented in Panakhov & Abbasov (2004), Panakhov & Omrani (2008). Here, first of all, we consider the conditions of additional stress state in the porous medium as a result of in situ gas formation, as well as elimination of complications associated with viscous instability and other complicating factors of the displacement process.

2 Experimental procedures

The laboratory studies were carried out on an experimental setup modelling the conditions of gas-generating solutions flow in porous medium. As a result of the experiments, it was determined that the pressure change in the reacting average and its maximum steady-state value of P as a result of stoichiometric reaction in solutions had different character and pressure change rate depending on the type of water used (Fig. 1). Dynamics of dissolution or diffusion of gas released as a result of the reaction also differed depending on the use of formation water or process water in the prepared solution. These results are in good agreement with the results of the authors Kristanto et al. (2020), Rodosta et al. (2017). Under the same thermodynamic conditions, rapid CO₂ release significantly changes the distribution of water and oil saturation in the displacement zone, as well as the volume flow rate in the boundary zone. In contrast to the experimental data, in the presence of porous medium the kinetics of gas generation has other features - at the initial stage of gas generation the pressure in the medium increases to a certain extreme value and then decreases. The process of gas release and pressure dynamics in this case has a non-equilibrium character - pressure growth in the system slows down the process of gas release and subsequent dissolution of the generated gas bubbles. This is shown in the Fig. 1, curves 1 and 2. In contrast, in the reaction medium with the use of the formation water as the aqueous phase in a porous medium, the pressure dynamics is monotonic (Fig. 1, curve 3).

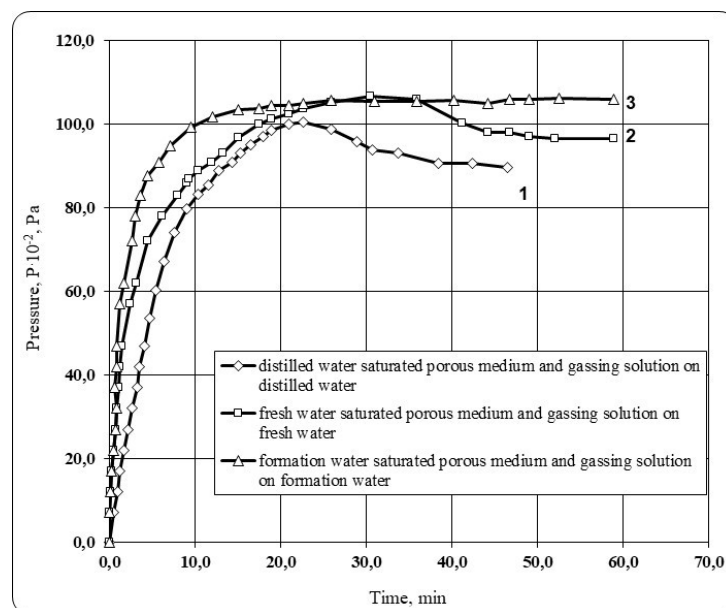


Figure 1: Pressure build-up curves on gas-generated solutions

3 Kinetics of gas generation

An exponential function equivalent to the first order linear differential equations used in the relaxation model is used to describe the gas release curve (Ferer & Smith, 1994). On the other hand, this approximation is made without taking into account all the details associated with the process, including the high mineralization of the fluids, as noted by Blunt et al. (1993), Chuoke et al. (1959), Li & Chen (2023). Therefore, a nonlinear kinetic model is used to describe gas separation.

If the reaction between solutions involves the factor of diffusion of additional gas into the medium, the pressure in this case rises to some extreme level and then begins to decrease. The correlation between gas release and pressure is non-equilibrium. Change of pressure leads to dissolution of gas in the medium after reaction (Fig. 2, curves 1 and 2). If in the reaction there is diffusion of additional gas into the medium, as noted by the authors Bakhtiyarov et al. (2006), Chukwuma (1983), Li et al. (2006), Riazi (1996), the pressure drop at the final stage of gas release is due to diffusion of gas bubbles from the medium into the liquid. In this case, the ratio of formation and dissolution of gas bubbles is written as follows:

$$\frac{dP}{dt} = a_1 - a_2P(t) - a_3P^2(t - \tau), \quad (1)$$

a_2 and a_3 – coefficients that take into account the gas dissolved in the liquid and already formed and diffused gas molecules; τ - is the characteristic diffusion time.

Let's consider the solution of the equation under the following conditions:

$$P(t) = \phi_0(t) \quad \text{at} \quad t_0 - \tau \leq t \leq t_0$$

$$\phi_0(t) = \frac{1}{2a\sqrt{\pi t}} e^{-\frac{x^2}{4a^2t}}; \quad (2)$$

$$\begin{cases} \frac{dP}{dt} = a_1 - a_2P(t) - a_3\phi_0^2(t - \tau) \\ t_0 \leq t \leq t_0 + \tau, \quad \rho(t_0) = \phi_0(t_0); \quad [t_0, t_0 + \tau] \end{cases} \quad (3)$$

The solution of the problem will be represented as the following function:

$$P_1(t) = e^{-a_2(t-t_0)}\phi_0(t_0) + \int_{t_0}^t e^{-a_2(t-s)} (a_1 - a_3\phi_0^2(s - \tau)) ds \quad (4)$$

$$\frac{dP}{dt} = a_1 - a_2P(t) - a_3P_1^2(t - \tau)$$

When

$$t_0 + \tau \leq t_0 \leq 2\tau, \quad P(t_0 + \tau) = P_1(t_0 + \tau) \quad (5)$$

$$\frac{\partial P}{\partial t} = a^2 \frac{\partial^2 P}{\partial x^2}, \quad t > 0, \quad P = \phi_0(t) \quad (6)$$

$$\phi_0(t, x) = \frac{1}{2a\sqrt{\pi t}} e^{-\frac{x^2}{4a^2t}}$$

$$\begin{aligned} P_1(t) &= e^{-a_2(t-t_0)} \cdot \frac{1}{2a\sqrt{\pi t_0}} e^{-\frac{x^2}{4a^2t_0}} + \int_{t_0}^t e^{-a_2(t-s)} a_1 ds - \\ &- \int_{t_0}^t e^{-a_2(t-s)} \cdot \frac{a_3}{4a^2\pi(s-\tau)} e^{-\frac{x^2}{2a^2(s-\tau)}} ds = \end{aligned}$$

$$\begin{aligned}
&= \frac{1}{2a\sqrt{\pi t_0}} \cdot e^{-a_2(t-t_0) - \frac{x^2}{4a^2 t_0}} + \frac{a_1}{a_2} \left(1 - e^{-a_2(t-t_0)}\right) - \int_{t_0}^t \frac{a_3}{4\pi(s-\tau)} \cdot e^{-a_2(t-s) - \frac{x^2}{2a^2(s-\tau)}} ds \\
P_1(t) &= \frac{a_1}{a_2} \left(1 - e^{-a_2(t-t_0)}\right) + \frac{1}{2a\sqrt{\pi t_0}} e^{-a_2(t-t_0) - \frac{x^2}{4a^2 t_0}} - \int_{t_0}^t \frac{a_3}{4\pi(s-\tau)} \cdot e^{-a_2(t-s) - \frac{x^2}{2a^2(s-\tau)}} ds. \quad (7)
\end{aligned}$$

According to Taylor's decomposition:

$$\begin{aligned}
e^{-a_2(t-s) - \frac{x^2}{2a^2(s-\tau)}} &= e_1^{-a_2(t-\tau)} \cdot e^{a_2(s-\tau)} \cdot e^{\frac{x^2}{2a^2(s-\tau)}} = \\
&= e^{-a_2(t-\tau)} \left(1 + a_2(s-\tau) + \frac{a_2^2}{2}(s-\tau)^2 + \dots\right) \left(1 - \frac{x^2}{2a^2(s-\tau)} + \frac{x^4}{4a^4(s-\tau)^2} - \dots\right) = \\
&= e^{-a_2(t-\tau)} \left(1 - \frac{a_2 x^2}{2a^2 t} + \left(a_2 - \frac{a_2^2 x^2}{4a^2}\right)(s-\tau) - \frac{x^2}{2a^2(s-\tau)}\right).
\end{aligned}$$

Further, in the first approximation

$$\begin{aligned}
P_1(t_1^T) &= \frac{a_1}{a_2} \left(1 - e^{-a_2(t-t_0)}\right) + \frac{1}{2a\sqrt{\pi t_0}} e^{-a_2(t-t_0) - \frac{x^2}{4a^2 t_0}} - \\
&- \frac{a_3}{4\pi} \left\{ \left(1 - \frac{a_2 x^2}{2a^2}\right) \ln \frac{t-\tau}{t_0-\tau} + \left(a_2 - \frac{a_2^2 x^2}{4a^2}\right) \cdot (t-t_0) + \frac{x^2}{2a^2} \frac{(t-t_0)}{(t-\tau)(t_0-\tau)} + \dots \right\}, \quad (8)
\end{aligned}$$

where,

$$a_1 = kv_1,$$

k – bubble formation rate; v_1 – bubble formation velocity;

$a_2 = \alpha v_2$ - coefficient that takes into account the relative solubility of the gas;

$a_3 = v_3$ - coefficient, which takes into account the influence of excessively generated gas on the formation of new bubbles.

4 Experimental estimation of carbon dioxide diffusion in fluid saturated porous media

Research on CO₂ diffusion in fluid-saturated porous media under reservoir conditions is very limited. For example, one of the most well-known difficulties is natural convection caused by the density increase in the liquid phase due to CO₂ dissolution, which greatly complicates the diffusion process, and traditional experimental schemes are considered unsuitable for measuring the CO₂ diffusion coefficient at high pressures (Li et al., 2006; Mandelbrot, 1982; Renner, 1988). To analyze the diffusion process (more precisely, self-diffusion, i.e. diffusion of molecules separated only from other particles in the medium), the free path length can be estimated by the following expression (Chukwuma, 1983; Li & Chen, 2023; Li et al., 2006):

$$\lambda = \frac{1}{\sqrt{2}\sigma n}$$

In the considered case it is assumed that average velocity of particles and velocities of diffusing particles are equal. If the z -axis in a porous medium is oriented orthogonal to the field S , and the other two axes x and y are parallel to the field, the randomness of molecular motion can be modelled as follows. Here it is assumed that exactly 1/3 of the molecules move along the x -axis, 1/3 along the y -axis and 1/3 along the z -axis. The molecules parallel to the z -axis (1/6 of the total number of molecules) move in the positive direction and the same number move in the negative direction, as it noted by Riazi (1996).

The expression for the gas particle flow can be written as follows:

$$\varphi(z) = \frac{dN}{dt} = -\frac{1}{3} \langle v \rangle \lambda \frac{\partial n(z)}{\partial z} S \quad (9)$$

Since this expression coincides with the first Fick's law in structure, the diffusion coefficient is defined as follows:

$$D = \frac{1}{3} \langle v \rangle \lambda \quad (10)$$

Given that $\lambda \sim \frac{1}{\sigma n} \sim \frac{T}{\sigma p}$, we can write the following expression:

$$D \sim \frac{1}{\sigma n} \sqrt{\frac{T}{\mu}} \sim \frac{T^{\frac{3}{2}}}{\sigma p \sqrt{\mu}}. \quad (11)$$

Since the 1930s, many studies of the gas diffusion coefficient in liquids have been carried out Bakhtiyarov et al. (2006), Chukwuma (1983), Dake (1998), Ferer & Smith (1994), Li & Chen (2023), Mandrik et al. (2010), Panakhov & Abbasov (2004), Panakhov & Omrani (2008), Li et al. (2006). Most of them were carried out using adsorption or diffusion PVT (pressure-volume-temperature) units. In this method, either the pressure changes in the system at constant volume, or the volume change of the gas phase at constant pressure, or both are detected as a function of time. The amount of gas diffusing in the liquid phase is calculated from the change in pressure or volume of the gas phase using the equation of state (EOS) of real gases (Astaniina & Sheremet, 2023; Upreti & Mehrotra, 2000). Grogan et al. proposed a glass capillary tube to measure the CO₂ diffusion coefficient in light oils under high pressure (Mirzaalian et al., 2023). A layer of CO₂ gas is created in the middle of the capillary tube filled with an oil sample. The position of the CO₂ and oil mixture in the tube is detected as a function of time to calculate the diffusion coefficient using a numerical model. Although this method can be used to measure the CO₂ diffusion coefficient in the liquid phase, it is difficult to apply it to saturated porous media, as the researchers pointed out, because some additional operations are required in the experiment to show the effect of convection on the measurement results (Mirzaalian et al., 2023).

Renner also found that the diffusion coefficient measured when the container was placed vertically was much greater than when it was placed horizontally due to the natural convection effect caused by the density in the previous situation where CO₂ diffused into the core sample from above (Li et al., 2006). The diffusion coefficient of a gas is determined by fitting the amount of gas diffusing into the liquid phase (or the change in pressure or volume of the gas phase) with time to appropriate diffusion models. The PVT method has been successfully used to measure diffusion coefficients of various gases in pressurized liquids, such as hydrocarbon gases, carbon dioxide CO₂ and nitrogen in oil and water (Li & Chen, 2023; Li et al., 2006; Riazi, 1996). The results of CO₂ diffusion coefficient determination obtained by the conventional PVT method may contain some errors. To overcome some drawbacks, the author Mirzaalian et al. (2023) presented a new method for measuring the effective CO₂ diffusion coefficient under reservoir conditions in oil-saturated porous media. A porous medium with two closed ends is considered as a physical model of the radial diffusion process. The measurement was carried out in a high-pressure diffusion chamber, in the middle of which a core sample saturated with oil was placed, and the rest of the field was filled with a high-pressure CO₂ sample. A mathematical model is proposed along with measurements as well as numerical solutions to describe these processes. The effective diffusion coefficient is determined by comparing the experimental pressure drop curve with the corresponding mathematical model (Mirzaalian et al., 2023). The method can be easily applied in laboratories capable of handling high-pressure fluids; thus, this study can be presented as a tool for research on CO₂ diffusion in oil-saturated porous medium.

5 Control of non-equilibrium state at the interface during gas conversion in a porous medium

Since the dissolution of these gases in the liquid reduces the density of the liquid phase, density-induced natural convection is not a concern. However, the PVT method cannot be used for most CO₂-liquid systems. This is because the dissolution of CO₂ in liquids such as oil and water lead to an increase in the density of the liquid phase. The density gradient can induce natural convection (Li & Chen, 2023; Li et al., 2006; Riazi, 1996). As a result, when the viscosity of the liquid phase is not high enough to balance the gravitational force caused by the density difference with the viscous force, the mass transfer of CO₂ into the liquid phase in the PVT method is inhibited or even controlled by density-driven convection (Saffman & Taylor, 1958; Upreti & Mehrotra, 2000). In studies modelling the unstable displacement of one fluid by another, the process of fractal structure formation is observed. Since the Hele-Shaw model (1899), numerous studies have attempted to determine the dynamics and geometry of the displacement front between one fluid and another (Mandelbrot, 1982). In Engelberts & Klinkenberg (1951) found that the boundary between two fluids has instability by conducting experiments on oil displacement by water in sandstone. Later Benoit Mandelbrot proved that many natural phenomena, including the formation of “viscosity columns”, have a fractal structure (Feder & Jossang, 1989; Mandelbrot, 1982; Niemeyer et al., 1984). It is known that when the injection pressure reaches a certain critical value of diffusion pressure during oil displacement by water in a porous medium, the displacing fluid advancement is observed. Later, stochastic growth of this phase occurs and a characteristic geometric pattern of different structures is formed in the medium. On the other hand, Feder (1988) and Smith (1994) have constructed a series of analytical and computer models that describe fractal growth in the special case of two-phase patterns (Feder & Jossang, 1989; Nazarov, 2021). Such an image allows to give the character of a geometric image with fractal dimensions and critical indicators. The realizable process is as follows: P_{\perp} is a non-conducting field and P_z is a conducting field. These parts (oil) are separated by stochastic shapes. It is interesting to determine the pressure P_z from this dependence. The probability of growth conditional on early gap satisfies Laplace’s equation. Taking into account, that $f(r, t)$ - is the probability of a random effect at a point r at time t , in this case U is the jump velocity, and $U \sim \nabla f$ is proportional to the local gradient of the growth probability between the search points. The rate of interface formation between the fluids is equal to the local pressure gradient, i.e. (Du et al., 2023; Iwasaki et al., 2023):

$$U_n = -n\nabla P \quad (12)$$

Taking into account the incompressibility condition (for Newtonian fluids), the Laplace equation for the pressure field can be written in the form:

$$\nabla^2 P = 0.$$

However, over a period of time, diffusion-limited compounds create non-fractally stable Saffman-Taylor lattices, leading to their mean-field limit as a result of the aggregate growth probability. Similarly, to surface tension, the mean-field limit causes a smoothing of the growth profile (Engelberts & Klinkenberg, 1951). However, it does not always prevent fractal growth. Fractal growth is observed in the presence of surface tension at the interface of two liquids, and the dimensions of the sample under consideration are many times larger than the critical growth wavelength. The wavelength is determined according to Chuoke et al. (1959):

$$\lambda = \frac{\pi b \sqrt{\sigma}}{\sqrt{U} \mu}, \quad (13)$$

b – crack thickness; v – speed of the front; μ - viscosity of the injected fluid; σ - surface tension at the separating boundary.

In the case of systems with non-Newtonian properties, where viscosity decreases with increasing shear rate, the above equations can be written as follows Zhuze et al. (1981):

$$\mu = c'\dot{\gamma}^{n-1}$$

$$\begin{aligned} U_n &= -n \left(|\nabla P|^{m-1} \nabla P \right) \\ \nabla \left(|\nabla P|^{m-1} \nabla P \right) &= 0 \end{aligned} \quad (14)$$

n' - velocity-dependent shear attenuation for the systems considered; $n' = 0, 4-0, 1$ (for polymer solutions).

Finding an analytical solution in the above system of equations allows us to draw certain conclusions about the growth of the mentioned process, which is solved as follows Saffman & Taylor (1958):

$$P(r) = \begin{cases} \frac{R^{(m-1)/m} - r^{(m-1)/m}}{R^{(m-1)/m} - 1}, & \text{at } m \neq 1 \\ 1 - \frac{\ln r}{\ln R}, & \text{at } m = 1 \end{cases} \quad (15)$$

$r = 1$, $P = 1$ and $r = R$,

under the boundary conditions $P = 0$. When $m = 1$, the velocity at the beginning of growth is proportional to $1/r$. An unstable structure can arise when $m < 1$ or $m > 1$, and the pressure field depends on the radius. The correctness of this assumption can be checked only by numerical solution of this equation. Here, the pressure changes P as a function of R at different values of m and n was considered and the following results were obtained (Fig. 2 ab).

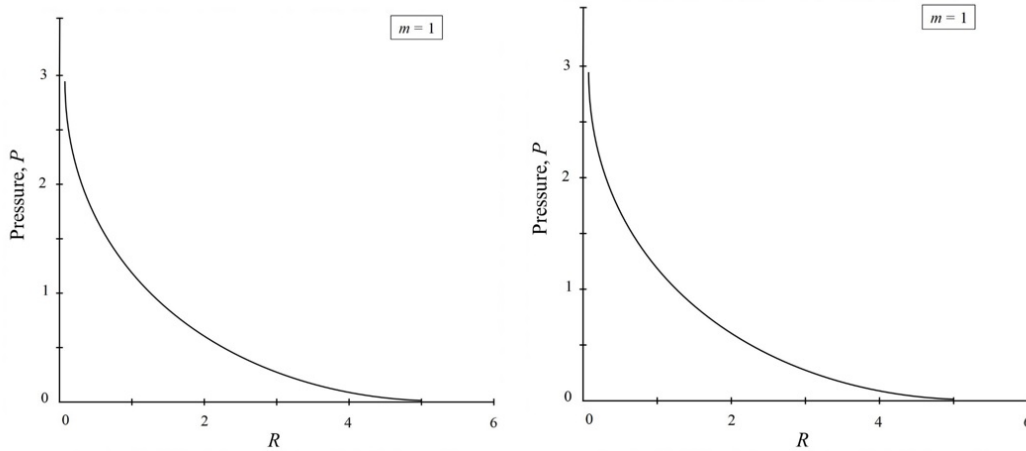


Figure 2: Dependence of pressure P vs. displacement front radius

As is known, non-equilibrium conditions (fluctuations) in the boundary layer between fluids in a porous medium and injected fluids can develop chaotically without experiencing the limiting effect of smoothing surface forces. Clearly, the densities and viscosities that can smooth the interface profile of the fluids are constant. Consequently, the transition from fractal to non-fractal growth can be characterized as a function of density and viscosity ratios (Mandelbrot, 1982). Growth is usually controlled by a global pressure field, and the competition between the growth of neighboring elements in the boundary layer between two fluids is proportional to the local pressure gradient. Such localized regions can also be associated with a process that leads to changes in viscosity and density of the fluids in the gas boundary layer between the displacing and displaced fluids. Under the same reservoir conditions, the density and viscosity of carbon dioxide are much lower than those of oil. Under certain special thermobaric conditions, carbon dioxide can also be in a supercritical state (Panahov et al., 2021; Mahmoodpour et al., 2023). In

the case of two fluids in a separate pore due to the free pressure drop gradient (Ferer & Smith, 1994) is defined as:

$$P_G = \rho_1 g a x \sin \phi + \rho_2 g (1 - a) x \sin \phi, \quad (16)$$

where:

a – the volume of the displaced liquid fraction;

$\rho_{1,2}$ – densities of displaced and displacing fluids;

g – acceleration due to gravitation force;

x – the distance between the centers of the pore channels;

φ – the angle between the channel axis and the horizontal axis.

In their work, the authors Dake (1998) propose the following expression for the free-fall pressure gradient in spherical pores filled with a two-phase system:

$$P_G = \rho_1 g \left(\frac{3\alpha}{4\pi} \right)^{1/3} \sin \psi + \rho_2 g \left[\left(\frac{3}{4\pi} \right)^{1/3} - \left(\frac{3\alpha}{4\pi} \right)^{1/3} \right] \sin \psi \quad (17)$$

where: ρ_1, ρ_2 – density of liquid; a – volume of displaced liquid fraction.

If, $\rho_1 = \rho_2 = \rho$, then

$$P_G = \rho g x \sin \phi.$$

When the gas phase is formed at the interface of the two phases and dissolved in the solutions, the parameters ρ_1 and ρ_2 will change:

$$P_G = \rho_1(t)k + \rho_2(t)(1 - k)$$

$$\rho_1 = \rho_2; P_G = \rho_{1,2} g x \sin x. \quad (18)$$

Further,

$$\begin{aligned} U_n &= -n \nabla P_1 \pm n \nabla P_2, \\ \nabla^2 P_1 \pm \nabla^2 P_2 &= 0. \end{aligned} \quad (19)$$

Under conditions $P_1 = P_2$, a stable pressure distribution occurs at the displacement boundary. The researchers found that density-viscosity ratios are directly proportional to the fractal dimension (Engelberts & Klinkenberg, 1951; Mandelbrot, 1982; Saffman & Taylor, 1958). Gas separation is a factor that significantly affects the boundary parameters (σ , ρ , μ) of the displacing and displacement-burning fluids and directly affects the absorption coefficient n .

6 Mathematical model of gas formation with diffusion and heat conduction effects

Carbon dioxide CO₂ mass transfer in a porous medium saturated with oil can be considered as a diffusion process combined with mass convection (volume expansion) in the radial direction in a one-dimensional radial system with a fixed location of the boundary and constant concentration (Mahmoodpour et al., 2023). Depending on the type of diffusion and taking into account, that both the velocity and concentration gradients in the directions θ and z are zero, the equation of concentration conservation can be written in scalar form as

$$\frac{\partial c}{\partial t} + \frac{c}{r} \frac{\partial}{\partial r} (ru) + u \frac{\partial c}{\partial r} = D_{eff} \nabla^2 c. \quad (20)$$

Equation (21) is a nonlinear partial differential equation. Because the coefficient (u velocity) in front of $(\partial c / \partial r)$ depends on the increase of diffusion concentration in the porous medium. For the inflatable system the velocity is zero (no convection), and then expression (21) simplifies to the following:

$$\frac{\partial c}{\partial t} = \frac{D_{eff}}{r} \frac{\partial}{\partial r} \left(r \frac{\partial c}{\partial r} \right). \quad (21)$$

Here, equation (21) is solved numerically. For such a system there are boundary conditions:

$$\begin{aligned} c &= c_0, & r &= r_0 \\ u &= 0, & \frac{\partial c}{\partial r} &= 0, & r &= 0 \end{aligned} \quad (22)$$

Initial conditions

$$\begin{aligned} u &= 0, & c &= c_i, & r &< r_0 \\ u &= 0, & c &= c_0, & r &= r_0, & t = 0 \end{aligned} \quad (23)$$

To measure the diffusion coefficient in that case, the liquid phase saturating the porous medium initially does not contain gas, i.e. $c_i = 0$ (Fig. 3).

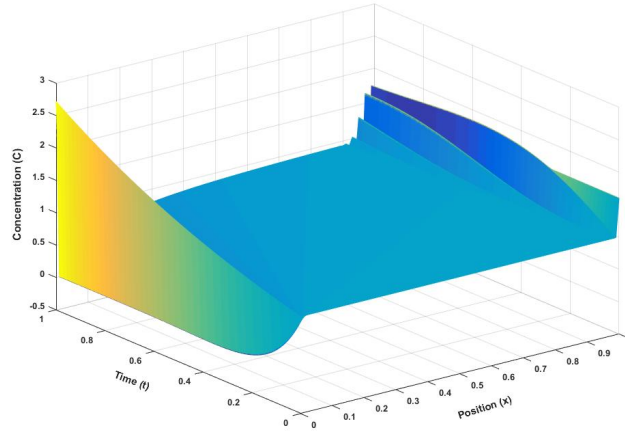


Figure 3: Gas-to-liquid diffusion coefficient estimation in fluid-saturated porous media

Let us consider the three-dimensional case of unsteady temperature distribution in a layer. The unsteady heat transfer equation for temperature $T(x, y, z, t)$ in a three-dimensional medium (x, y, z) is written as follows:

$$\frac{\partial T}{\partial t} = \alpha \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right), \quad (24)$$

where α is the heat transfer coefficient. To ensure the stability of the numerical solution of equation (24), an unknown finite difference scheme was used. The scheme of the unknown finite difference method for this equation is as follows Zhuze et al. (1981):

$$\begin{aligned} \frac{T_{i,j}^{n+1} - T_{i,j}^n}{\Delta t} &= \alpha \left(\frac{T_{i-1,j}^n - 2T_{i,j}^{n+1} + T_{i+1,j}^n}{\Delta x^2} + \frac{T_{i,j-1}^n - 2T_{i,j}^{n+1} + T_{i,j+1}^n}{\Delta y^2} \right). \quad (25) \\ &= \alpha \left(\frac{T_{i-1,j,k}^n - 2T_{i,j,k}^{n+1} + T_{i+1,j,k}^n}{\Delta x^2} + \frac{T_{i,j-1,k}^n - 2T_{i,j,k}^{n+1} + T_{i,j+1,k}^n}{\Delta y^2} + \frac{T_{i,j,k-1}^n - 2T_{i,j,k}^{n+1} + T_{i,j+1,k+1}^n}{\Delta z^2} \right). \end{aligned}$$

From equation (25), the value of $T_{i,j}^{n+1}$ ($T_{i,j,k}^{n+1}$) is determined as follows:

$$T_{i,j}^{n+1} = \frac{T_{i,j}^n + A \left(T_{i-1,j}^n + T_{i+1,j}^n \right) + B \left(T_{i,j-1}^n - T_{i,j+1}^n \right)}{2(A+B)}, \quad (26)$$

$$T_{i,j,k}^{n+1} = \frac{T_{i,j,k}^n + A \left(T_{i-1,j,k}^n + T_{i+1,j,k}^n \right) + B \left(T_{i,j-1,k}^n - T_{i,j+1,k}^n \right) + C \left(T_{i,j,k-1}^n - T_{i,j,k+1}^n \right)}{2(A+B+C)},$$

where,

$$A = \frac{\alpha \cdot \Delta t}{\Delta x^2}, \quad B = \frac{\alpha \cdot \Delta t}{\Delta y^2}, \quad C = \frac{\alpha \cdot \Delta t}{\Delta z^2}.$$

The scheme used is certainly stable. The basic steps were as follows. The number of calculation points in the transverse direction was 100 x 100. The harmonic law of temperature change during gas formation was assumed. This is justified, firstly, by the fact that real profiles differ insignificantly from harmonic profiles and, secondly, by reducing the depth of penetration of higher harmonics into the array. If we define the heat conduction equation for a half-space with a certain boundary condition of the temperature field in the surrounding medium, only provided that the temperature is bounded by infinity in the vertical direction, we obtain:

$$\begin{aligned} \frac{\partial T}{\partial t} &= \chi \frac{\partial^2 T}{\partial z^2} \\ z = 0 : T &= T_0 + \theta_0 \cos(\omega t), \\ z \rightarrow \infty : T &< \infty \end{aligned} \quad (27)$$

where T_0 - average temperature, θ_0 - amplitude of temperature fluctuations, χ - thermal conductivity of the array, $2\pi/\omega$ - time period, the vertical coordinate is calculated by gas formation in the direction of displacement. Thus, the following temperature distribution occurs in the array:

$$T = T_0 + \theta_0 e^{-kz} \cos(\omega t - kz), \quad k = \sqrt{\frac{\omega}{2\chi}}. \quad (28)$$

To complete the mathematical formulation of the problem, only the temperature dependence of the molecular diffusion coefficient is taken into account Astanina & Sheremet (2023):

$$D_{mol} = \frac{k_B T}{2\pi\mu R} \cdot \frac{\mu + \nu}{2\mu + 3\nu}. \quad (29)$$

Here Boltzmann constant is the dynamic viscosity of a liquid in which molecules of a certain size are distributed. The value of the parameter determined as a result of experimental studies (Astanina & Sheremet, 2023; Zhang et al., 2000) was as follows:

$\nu = 5.47 \cdot 10^{-5}$ Pa.s. Equation (29) describes molecular diffusion without taking into account other effects when the average free path length corresponds to the pore size (Astanina & Sheremet, 2023). Using this expression, the variation of the above parameters depending on each other is estimated (Fig. 4).

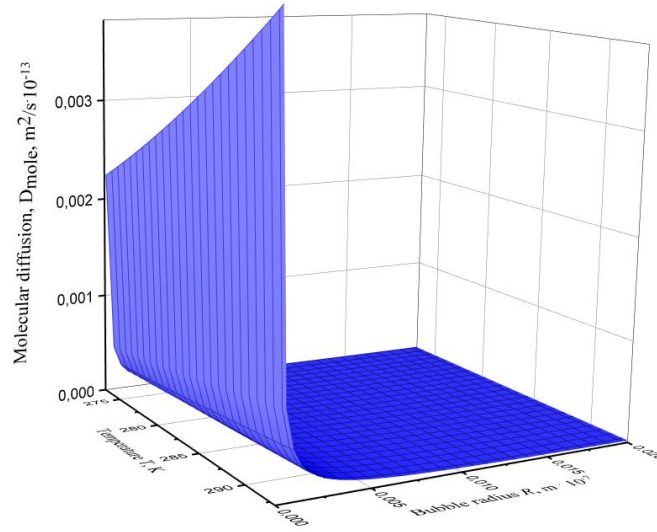


Figure 4: 3D dependence of molecular diffusion D vs. temperature T vs. bubble radius R

Next, the joint estimation of diffusion and heat transfer in gas formation is considered. Here, the effect of temperature and diffusion boundaries (fronts) in a chemical reaction is taken into account. In this case, the differential equation can be written as follows.

$$\begin{aligned} \frac{\partial C}{\partial t} &= D(T) \frac{\partial^2 C}{\partial x^2} - k(T) C^n; \\ \alpha\beta \frac{\partial T}{\partial t} &= \gamma \frac{\partial^2 T}{\partial x^2} + q_T + k(T) C^n. \end{aligned} \quad (30)$$

For simplicity, we write equations (30) in the form:

$$\begin{aligned} \frac{\partial C}{\partial t} &= D(T) \frac{\partial^2 C}{\partial x^2} \\ \alpha\beta \frac{\partial T}{\partial t} &= \gamma \frac{\partial^2 T}{\partial x^2}. \end{aligned} \quad (31)$$

After appropriate replacement we pass in these equations to polar coordinates:

$$\begin{aligned} \frac{\partial C}{\partial t} &= D(T) \left(\frac{\partial^2 C}{\partial r^2} + \frac{2}{r} \frac{\partial C}{\partial r} \right) \\ \frac{\partial T}{\partial t} &= \frac{\gamma}{\alpha\beta} \left(\frac{\partial^2 T}{\partial r^2} + \frac{2}{r} \frac{\partial T}{\partial r} \right), \end{aligned} \quad (32)$$

where $D(t)$ and $\frac{\gamma}{\alpha\beta}$ are the thermal diffusivity and diffusion coefficients.

We consider that at the initial point in time, a saturation state is instantly established on the entire surface of the gas bubble, which is further kept during the entire heat and mass transfer process and is characterized by a linear dependence of the concentration of the target component on temperature. According to the assumptions, let us write down the initial and boundary conditions:

$$C(r_1) \Big|_{t=0} = C_0(r) \quad (33)$$

$$T(r) \Big|_{t=0} = T_0(r) \quad (34)$$

$$T(r=R, t) = \partial T(r=R, t) \quad (35)$$

$$\lambda_p \left(\frac{\partial C}{\partial r} \right)_{r=R} = r_p \frac{\gamma}{\alpha\beta} \left(\frac{\partial T}{\partial r} \right)_{r=R} \quad (36)$$

$$C(r = R, t) = e^r \quad (37)$$

$$T(r = R) = T^2 \quad (38)$$

Using the Fourier method, we have the solution:

$$C(r) = \frac{2R}{r} \frac{\alpha_1}{\sqrt{\pi}} \int_0^{(r-R)/2\sqrt{Dt}} e^{-x^2} dx + \frac{R}{r} C_0(r) \quad (39)$$

$$T(r) = \frac{2R}{r} \frac{\alpha_2}{\sqrt{\pi}} \int_0^{(r-R)/2\sqrt{Dt}} e^{-x^2} dx + \frac{R}{r} T_0(r). \quad (40)$$

7 Conclusion

Experimental studies have provided an estimation of the pressure change under the gas formation in the porous medium (under reservoir conditions). It is shown that the process can be described by a nonlinear dependence with a lagging argument.

The dynamics of the gas formed in the porous medium and the effects accompanying the gas formation process were evaluated. The influence of the process on gas diffusion and heat and mass transfer effects was revealed.

Mathematical modelling of the convection of the formed gas phase revealed that the heat and mass transfer process is characterised by CO₂ diffusion in the gas-liquid medium and is expressed by a linear dependence of gas concentration on temperature.

It was found that strong exponential dependence of solubility and molecular diffusion coefficient on temperature leads to instantaneous diffusion flows of generated gas into porous medium saturated with liquid. In-situ gas generation can provide a method to control the non-equilibrium fractal state at the interface during displacement in a porous medium.

Effect is manifested in the increase of the hydrocarbon displacement coefficient due to the levelling of the densities of the displacing and displaced agents, as a consequence of the increase in gas saturation of the fluid. Investigate matters can provide an effective way to hydrocarbons recover from oil saturated reservoirs.

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