NUMERICAL MODEL OF MASS TRANSFER IN POROUS MEDIUM

YAROSLAV DANILOVYCH P'YANYLO
AND NAZARIY BOGDANOVYCH LOPUH

Centre for Mathematical Modelling,
Pidstryhacha Institute for Applied Problems of Mechanics and Mathematics,
Ukrainian Academy of Science,
Dudajev str. 15, 79005 Lviv, Ukraine
pjanylo@cmm.lviv.ua

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Abstract: A new numerical model of gas filtration in a porous medium is proposed and investigated. Gas filtration is modeled with a nonlinear differential equation in partial derivatives. Methods of solving the equation are discussed. A computer experiment basing on real-experiment-extracted input physical and geometrical parameters is performed and its results are analyzed. The received results agree well with the corresponding experimental data.

Keywords: gas filtration, finite element method, discretization

1. Introduction

A significant number of works in the literature is devoted to the research on porous media [1]. In nature porous environments are carriers of hydrocarbons, water and many other useful substances. Adequate mathematical models of porous environments allow developing algorithms for their optimal design and operation [2, 3]. As a rule, mass transfer in porous media is described by nonlinear differential equations in partial derivatives or systems of such equations. Since the input parameters and the properties of the porous medium are usually known with low accuracy, an accurate solution of the modeled mathematical and physical problems presents considerable computing difficulties. Exact analytical solutions exist merely in few cases. Numerical and iterative methods or linearization of the initial equations are basically used to obtain approximate solutions. It is worth noting that the linearization of equations often gives solutions sufficiently accurate for many practical problems. Adequacy and reliability of these solutions substantially depends on the linearization method. In this work, the effect of the method of linearization of the initial equation on the adequacy and accuracy of the obtained solution is investigated on the example of modeling of gas filtration in a porous medium. A comparison of the numerical and experimental results is a criterion of the mentioned adequacy and reliability of the chosen numerical scheme.

The finite elements method (FEM) is a widespread method of solving problems of the abovementioned type. In [4] this method is used for setting the initial boundary conditions on the set of the measured discrete data. As each numerical method, the FEM has also its specific features and limitations. As the initial equation is nonlinear, a direct application of the FEM leads to the necessity of solving high order nonlinear systems of algebraic equations. If the starting equation is initially linearized, then the linearization error is near to the FEM error. Thus, the accuracy of the solution method chosen for the corresponding problem of mathematical physics should be compatible with the expected overall accuracy.

2. Model of gas filtration in porous environment

The mass transfer in porous medium is exemplified here as gas and fluid filtration, described by the following equation:

$$\frac{\partial}{\partial x}\left(\frac{kh}{\mu z}\frac{\partial p^l}{\partial x}\right)+\frac{\partial}{\partial y}\left(\frac{kh}{\mu z}\frac{\partial p^l}{\partial y}\right)+\frac{\partial}{\partial c}\left(\frac{kh}{\mu z}\frac{\partial p^l}{\partial c}\right)=2mh\left(\frac{\partial}{\partial t}\left(\frac{p}{z}\right)+2qp_{at}\right) \qquad (1)$$

In Equation (1) $l=2$ for gas, and $l=1$ for an incompressible fluid; $k=k(x,y,c,t)$, $m=m(x,y,c)$ and $h=h(x,y,c)$ are the coefficient of permeability, porosity and thickness of the considered medium, respectively; μ is dynamic viscosity of gas, p_{at} pressure, q density, z the gas compressibility coefficient, for calculation of which a significant number of empirical formulas based on experimental data is used including:

$$z=\frac{1}{1+fp} \qquad (2)$$

where $f=(24-0.21t°\mathrm{C})\cdot 10^4$, and pressure $p(x,y,c)$ is measured in atmospheres; x, y, c are spatial Cartesian coordinates; t is the time. Gas is extracted from porous medium through I wells located at points (x_i^0,y_i^0,c_i^0), active during certain periods of time $t\in[t_{1i},t_{2i}]$, $(i=\overline{1,I})$. Therefore, the extraction density is determined by the formula:

$$q=\frac{1}{V}\sum_{i=1}^{I}q_i(x,y,c,t)\delta(x-x_i^0t)\delta(y-y_i^0)\delta(c-c_i^0)\left[\eta(t-t_{1i})-(t-t_{2i})\right] \qquad (3)$$

Here q_i is the extraction from the i-th well at the moment t, $\delta(x)$ is the delta-function, $\eta(t-t_{ji})$ is the Heaviside unit-step function.

The main problem is to find the solution $p(x,y,c,t)$ of Equation (1) for known values of pressure $p(x_i,y_i,c_i,t_0)$ at given points of the medium. The criteria of the adequacy and reliability of the solution are: the pressure values in the metering and monitoring wells and the condition gas mass balance in the medium, defined by the formula:

$$M = \int_V \rho dv \tag{4}$$

where integration iscarried out the storage volume V, M is the mass of gas in storage, ρ density under pressure equation of state, $p = \rho z R T$. Here R is the gas constant and T is the gas temperature. Note that it is not the mass of gas in the medium that is actually measured, but the mass changes ΔM at subsequent instants of time:

$$\Delta M = \int_V \Delta\rho dv = \int_V \frac{\Delta p}{\Delta z \Delta R \Delta T} dv \tag{5}$$

ΔM values are thus determined by the calculated pressure drops.

3. Problem formulation

It is known from geological investigations that the gas and oil carrying layers usually have an insignificant thickness (an order of several tens of meters) and considerable sizes in horizontal directions (several square kilometers). In most cases layers are almost horizontal. In the case of gas-carrying layers the gas pressure difference between the top and bottom surfaces of a layer is insignificant. Thus, at gas selection-pumping through vertical chinks, the layer can be vertically averaged over pressure and thus considered as two-dimensional.

Let $\Omega \subset \mathbb{R}^2$ be a two-dimensional region occupied by a porous medium. Within Ω, let a set of points (set of wells) with coordinates $\{x_i, y_i\}$, $i = 1, \ldots, n$, and the pressures values of $p(x_i, y_i, t_0)$ at these points be given at time t_0. Denoting:

$$\tilde{k}_x = k_x / k_c, \quad \tilde{k}_y = k_y / k_c \tag{6}$$

the distribution of gas pressure $p(x, y, t)$ in a layer in a non-stationary case is described by the following nonlinear differential equation in partial derivatives:

$$\frac{\partial}{\partial x}\left(\frac{\tilde{k}_x h}{\mu z}\frac{\partial p^2}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{\tilde{k}_y h}{\mu z}\frac{\partial p^2}{\partial y}\right) = 2\alpha_n m h \frac{\partial}{k_c \partial t}\left(\frac{p}{z}\right) + \frac{4}{k_c} m h q p_{st} \tag{7}$$

where k_u is the layer permeability in the u direction α_n is the gas saturation. Parameters of Equation (7) depend on the spatial coordinates and time. The dependences are unknown and it is necessary to build inverse problems for their development. The solution of such problems involves considerable difficulties. However, in practice the changes of parameters are negligible and can be considered constant in certain space-timeregions.

Equation (7) on the border Γ_2 of the Ω region (Figure 1) satisfies the Neumann boundary condition:

$$\Phi p(x, y) = 0, \quad (x, y) \in \Gamma_2 \tag{8}$$

where

$$\Phi p \stackrel{def}{=} \frac{kh}{\mu z}\frac{\partial p}{\partial x}\nu_x + \frac{kh}{\mu z}\frac{\partial p}{\partial y}\nu_y; \quad \nu_x = \cos(\nu, x), \;\; \nu_y = \cos(\nu, y) \tag{9}$$

and the boundary condition at Ω_*:

$$p(x_i, y_i, t^j) = p_1, \quad (x_i, y_i) \in \Omega_* \tag{10}$$

Here Γ_2 is the external border of region Ω; Ω_* is a subset of Ω including the points with known values of pressure p_i^j, j is the time index; ν is the external vector normal to the region $\Omega \subset \mathbb{R}^2$.

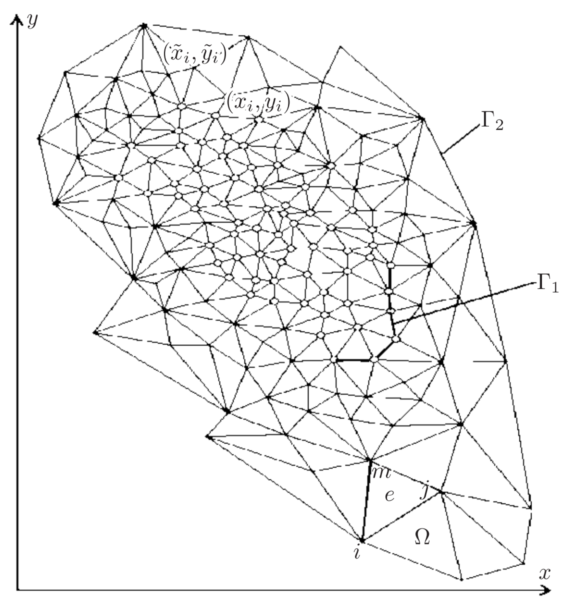

Figure 1. Exemplary triangulation of porous medium

Since there is no transport of gas across border Γ_2, the pressure gradient along the vector normal to the boundary vanishes and $\frac{\partial p}{\partial n} = 0$ should be taken as a boundary condition. In order to find analytical solution to define the initial distribution of the reservoir pressure. Taking the end of the neutral period as a reference point, the initial pressure distribution can be assumed to be constant and equal to the measured value, p_0.

4. Iterative schemes for layer pressure calculation

Let us rewrite Equation (1) in the following form:

$$\frac{\partial}{\partial x}\left(\frac{kh}{\mu z} p \frac{\partial p}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{kh}{\mu z} p \frac{\partial p}{\partial y}\right) = mh\left(\frac{\partial}{\partial t}\left(\frac{p}{z}\right) + 2qp_{at}\right) \tag{11}$$

It is known from experimental data that, when operating underground, the change rate of the reservoir pressure in an underground gas storage is small. Therefore, Equation (11) can be linearized as follows:

1. Let p_* be the pressure at the previous iterative step. Then Equation (11) can be written in the form:

$$\frac{\partial}{\partial x}\left((p-p_*+p_*)\frac{\partial p}{\partial x}\right)+\frac{\partial}{\partial y}\left((p-p_*+p_*)\frac{\partial p}{\partial y}\right)=\frac{m\mu}{k}\frac{\partial p}{\partial t}+\frac{2}{k}m\mu z p_{at}q \tag{12}$$

From which it follows that:

$$\frac{\partial^2 p}{\partial x^2}+\frac{\partial^2 p}{\partial y^2}=\frac{m\mu}{kp_*}\frac{\partial p}{\partial t}+\frac{2p_{at}}{kp_*}m\mu zq+\delta(x,y,p) \tag{13}$$

with

$$\delta(x,y,p)=\frac{\partial}{\partial x}\left((p-p_*)\frac{\partial p}{\partial x}\right)+\frac{\partial}{\partial y}\left((p-p_*)\frac{\partial p}{\partial y}\right) \tag{14}$$

If $p^{(j)}$ is the j-th approximation of the solution, the iterative procedure is defined as:

$$\frac{\partial^2 p^{(j)}}{\partial x^2}+\frac{\partial^2 p^{(j)}}{\partial y^2}=\frac{m\mu}{kp_*}\frac{\partial p^{(j)}}{\partial t}+\frac{2p_{at}}{kp_*}m\mu zq+\delta(x,y,p^{(j-1)}) \tag{15}$$

Multiplying the above equation by $\frac{kp_*}{m\mu}=\kappa_1$ one obtains:

$$\frac{\partial p^{(j)}}{\partial t}-\kappa_1\left(\frac{\partial^2 p^{(j)}}{\partial x^2}+\frac{\partial^2 p^{(j)}}{\partial y^2}\right)=-2kp_{at}zq-\kappa_1\delta\left(x,y,p^{(j-1)}\right) \tag{16}$$

Denoting:

$$\psi(x,y,z)=-2kzp_{at}q \tag{17}$$

the linearized equation for the pressure distribution of gas or liquid in complex porous medium becomes:

$$\frac{\partial p}{\partial t}-\kappa_1\left(\frac{\partial^2 p}{\partial x^2}+\frac{\partial^2 p}{\partial y^2}\right)=\psi(x,y,z) \tag{18}$$

2. Linearization of the left hand side of Equation (11) gives:

$$\frac{\partial}{\partial x}\left(\frac{kh}{\mu z}\frac{\partial p^2}{\partial x}\right)\approx 2\frac{kh}{\mu z}p_*\frac{\partial}{\partial x}\left(\frac{\partial p}{\partial x}\right)+2\frac{\partial}{\partial x}\left(\frac{kh}{\mu z}p_*\right)\frac{\partial}{\partial x}(p_*) \tag{19}$$

$$\frac{\partial}{\partial y}\left(\frac{kh}{\mu z}\frac{\partial p^2}{\partial y}\right)\approx 2\frac{kh}{\mu z}p_*\frac{\partial}{\partial y}\left(\frac{\partial p}{\partial y}\right)+2\frac{\partial}{\partial y}\left(\frac{kh}{\mu z}p_*\right)\frac{\partial}{\partial y}(p_*) \tag{20}$$

On the right hand side of Equation (11) parameter z is factored out from the derivative as a constant:

$$\frac{\partial}{\partial t}\left(\frac{p}{z}\right)\approx\frac{1}{z}\frac{\partial}{\partial t}(p) \tag{21}$$

Thus, the linearized version of Equation (11) reads:

$$p_*\frac{kh}{\mu z}\frac{\partial}{\partial x}\left(\frac{\partial p}{\partial x}\right)+p_*\frac{kh}{\mu z}\frac{\partial}{\partial y}\left(\frac{\partial p}{\partial y}\right)=\alpha mh\frac{1}{z}\frac{\partial}{\partial t}(p)+2mhqp_{st}+F(p_*,k,h,mu,z) \tag{22}$$

where

$$F(p_*,k,h,mu,z)=-\frac{\partial}{\partial x}\left(\frac{kh}{\mu z}p_*\right)\frac{\partial p_*}{\partial x}-\frac{\partial}{\partial y}\left(\frac{kh}{\mu z}p_*\right)\frac{\partial p_*}{\partial y} \tag{23}$$

We apply iteratively the finite element method combined with the difference scheme of time discretization to construct a numerical model of non-stationary problems of gas filtration in a porous medium. During the calculations the linearized version of Equation (11) is solved iteratively at each time interval.

3. Another numerical-analytical scheme is as follows. Let us introduce the notation $p^2=f$ in:

$$\frac{\partial}{\partial x}\left(\frac{k_x h}{\mu z}\frac{\partial p^2}{\partial x}\right)+\frac{\partial}{\partial y_1}\left(\frac{k_{y_1} h}{\mu z}\frac{\partial p^2}{\partial y_1}\right)+\frac{\partial}{\partial y_2}\left(\frac{k_{y_2} h}{\mu z}\frac{\partial p^2}{\partial y_2}\right)=2\alpha_n mh\frac{\partial}{\partial t}\left(\frac{p}{z}\right)+4mhqp_{st} \tag{24}$$

Despite the fact that the parameters of the latter equation depend also on the coordinates and on time, it follows from computational experiments that the parameters can be equally appropriately considered as variable, or averaged using iterative refinement. Let us consider the latter option. In such event:

$$\frac{\partial^2 f}{\partial x^2}+\frac{\partial^2 f}{\partial y_1^2}+\frac{\partial^2 f}{\partial y_2^2}=2\alpha_n m\frac{\mu}{k_x}\frac{\partial\sqrt{f}}{\partial t}+\frac{\mu z}{k_x}4mqp_{st} \tag{25}$$

Integrating the above in respect of time from t_1 to t_2 one obtains:

$$\begin{gathered}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y_1^2}+\frac{\partial^2}{\partial y_2^2}\right)\int_{t_1}^{t_2} f dt=2\alpha_n m\frac{\mu}{k_x}\left(\sqrt{f(x,y_1,y_2,t_2)}-\sqrt{f(x,y_1,y_2,t_1)}\right)+\\ +\frac{\mu z}{k_x}4mp_{st}\int_{t_1}^{t_2} q dt\end{gathered} \tag{26}$$

Approximating the integral on the left hand side of the latter equality with the trapezoid formula one obtains:

$$\int_{t_1}^{t_2} f dt=\frac{t_2-t_1}{2}\left[f(x,y_1,y_2,t_2)+f(x,y_1,y_2,t_1)\right]=\frac{t_2-t_1}{2}\psi(x,y_1,y_2,t_1,t_2) \tag{27}$$

We can assume that the outflow density is a known function. In such event the integral on the right hand side has a parametric representation:

$$\int_{t_1}^{t_2} q dt=q_1(x,y_1,y_2,t_1,t_2)\equiv q_1 \tag{28}$$

It is known that the reservoir pressure changes only slighty in time. Therefore, we can decompose the $\varphi=\sqrt{f}$ function in a Taylor series time variable t in the neighborhood of $t=t_1$, taking only the first two terms:

$$\varphi=\sqrt{f(x,y_1,y_2,t_2)}=\sqrt{f(x,y_1,y_2,t_1)}+\frac{f_t'(x,y_1,y_2,t_1)}{2\sqrt{f(x,y_1,y_2,t_1)}}(t_2-t_1) \tag{29}$$

from which it follows that:

$$\sqrt{f(x,y_1,y_2,t_2)}-\sqrt{f(x,y_1,y_2,t_1)}=\frac{f_t'(x,y_1,y_2,t_1)}{2\sqrt{f(x,y_1,y_2,t_1)}}(t_2-t_1) \tag{30}$$

Thus, in order to determine the f function the following equation is obtained:

$$\frac{t_2-t_1}{2}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y_1^2}+\frac{\partial^2}{\partial y_2^2}\right)\psi(x,y_1,y_2,t_1,t_2)=\alpha_n m\frac{\mu}{k_x}\frac{f_t'(x,y_1,y_2,t_1)}{\sqrt{f(x,y_1,y_2,t_1)}}(t_2-t_1)+ \\ +\frac{\mu z}{k_x}4mp_{st}q_1(x,y_1,y_2,t_1,t_2) \tag{31}$$

or

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y_1^2}+\frac{\partial^2}{\partial y_2^2}\right)\psi(x,y_1,y_2,t_1,t_2)=2\alpha_n m\frac{\mu}{k_x}\frac{f_t'(x,y_1,y_2,t_1)}{\sqrt{f(x,y_1,y_2,t_1)}}+ \\ +\frac{8mp_{st}\mu z}{(t_2-t_1)k_x}q_1(x,y_1,y_2,t_1,t_2) \tag{32}$$

We can assume that the function $f(x,y_1,y_2,t_1)$ and its derivative are known at the first step of the iteration procedure. At subsequent steps:

$$f_t'(x,y_1,y_2,t_2)=\frac{f(x,y_1,y_2,t_2)-f(x,y_1,y_2,t_1)}{t_2-t_1} \tag{33}$$

Then

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y_1^2}+\frac{\partial^2}{\partial y_2^2}\right)[f(x,y_1,y_2,t_2)+f(x,y_1,y_2,t_1)]= \\ =\frac{2\alpha_n m\mu}{k_x\sqrt{f(x,y_1,y_2,t_1)}}\frac{f(x,y_1,y_2,t_2)-f(x,y_1,y_2,t_1)}{t_2-t_1}+\frac{8mp_{st}\mu z}{(t_2-t_1)k_x}q_1(x,y_1,y_2,t_1,t_2) \tag{34}$$

The iterative procedure of determining the unknown function $f(x,y_1,y_2,t)$ is based on the latter equation. If the value of t_2-t_1 in the latter formulas coincides with Δt in the method of finite elements, then the latter equation is equivalent to:

$$\frac{\partial^2 f}{\partial x^2}+\frac{\partial^2 f}{\partial y_1^2}+\frac{\partial^2 f}{\partial y_2^2}=\alpha_n m\frac{1}{\sqrt{f_*}}\frac{\mu}{k_x}\frac{\partial\sqrt{f}}{\partial t}+\frac{\mu z}{k_x}4mqp_{st} \tag{35}$$

where f_* is the iterative approximate value of f.

5. Finite element method

The two-dimensional region Ω (Figure 1) is divided into elementary triangular elements [5]. The domain triangulation is performed in such a way that the coordinates of the known values of pressure (x_i,y_i) coincide with the coordinates of the triangle vertices. $(\tilde{x}_i,\tilde{y}_i)$ are the triangle vertices at which the pressure values are to be found.

In general, the differential equation in partial derivatives of the second order is written as:

$$-\sum_{i,j=1}^{2}\frac{\partial}{\partial x_i}\left(a_{ij}(x)\frac{\partial u}{\partial x_j}\right)+gu=f, \quad x\in\Omega_2\subset\mathbb{R}^2 \tag{36}$$

$$u(x_{1i},x_{2i},t^j)=u_i^j,\quad (x_{1i},x_{2i})\in\Omega_* \tag{37}$$

$$\Phi u(x)=0,\quad x\in\Gamma_2 \tag{38}$$

where u is the unknown function and a_{ij}, g, f are functions continuous in the domain. Finding a generalized solution of problem (36)–(38) consists in minimization of the functional:

$$F(u)=\int_\Omega \sum_{i,j=1}^{2} a_{ij}\frac{\partial u}{dx_i}\frac{du}{dx_j}dx+\int_\Omega gu^2dx-2\int_\Omega fu\,dx \tag{39}$$

Approximate solution u_h of the variational problem is sought in the form of $u_e=N_eq_e$, where $N_e=(\varphi_i,\varphi_j,\varphi_m)$ is the matrix of the basis functions; $q_e=(u_i,u_j,u_m)^T$ is the matrix of values of the sought solution at the vertices of triangular elements. Superscript T means the transpose operation, and the index e – an elementary triangle.

The basis functions for triangular elements are chosen as:

$$\varphi_i(x_1,x_2)=\frac{1}{2S_e}(a_i+b_ix_1+c_ix_2) \tag{40}$$

where S_e is the area of the triangle, and the coefficients a_i, b_i, c_i are determined by the coordinates of the triangle vortices.

From the variational formulation (39) we obtain a system of linear algebraic equations:

$$\sum_j u_j(A\varphi_i,\varphi_j)=(f,\varphi_j),\quad i,j=1,\dots,n \tag{41}$$

The linearized differential Equations (18) and (22) are reduced to Equation (39) using an explicit scheme of discretization in time:

$$\frac{\partial u}{\partial t}\approx\frac{u_t-u_{t-1}}{\Delta t} \tag{42}$$

where Δt is the step of discretization in time, u_{t-1} is the value of the solution received at the previous time step. The above described FEM scheme is used iteratively for linearized equations at each time step.

6. Calculation

The proposed scheme was tested in the numerical experiment performed on a porous medium of an area of $S=16\,\mathrm{M\,m^2}$, with the following initial parameters: $\mu=0.000011\,\mathrm{Pa\cdot s}$, $h=18.2\,\mathrm{m}$, $R=506.7\,\mathrm{J/kg\cdot K}$, $T=293\,\mathrm{K}$, $z=0.87$, $m=0.31$, $k=1.8\cdot10^{-12}\,\mathrm{m^2}$. The input information was provided by the values of pressure in control, measurement and operating wells in the neutral period. The reservoir pressure distribution was determined over a period of gas extraction (six months).

Tables 1 and 2 show the calculated values of the average reservoir pressure (P_{pl}) for various times (t). In the left column of the table 'No.' corresponds to the number of the linearization method (see Section 4) used in the computational scheme, ΔP_i is the difference between the measured values, P_z, and the corresponding calculated values.

Table 1. Values of average reservoir pressure P_{pl} t days after beginning of gas extraction from storage, $\Delta t = 1$ day

Method	P_{pl} (atm)						
	$t=0$	$t=30$	$t=60$	$t=90$	$t=120$	$t=150$	$t=180$
No. 1	51.54	47.78	43.99	38.57	33.74	29.31	28.99
No. 2	51.54	47.90	44.05	39.16	33.98	29.64	29.28
No. 3	51.54	47.37	43.58	38.26	34.18	29.86	29.69
ΔP_1	0.02	−0.59	−0.86	−0.29	0.39	0.47	0.59
ΔP_2	0.02	−0.71	−0.92	−0.88	0.15	0.14	0.3
ΔP_3	0.02	−0.38	−0.45	0.02	−0.05	−0.08	−0.11
P_z (atm)	51.56	47.19	43.13	38.28	34.13	29.78	29.58

Table 2. Values of average reservoir pressure P_{pl} t days after beginning of gas extraction from storage, $\Delta t = 0.5$ day

Method	P_{pl} (atm)						
	$t=0$	$t=30$	$t=60$	$t=90$	$t=120$	$t=150$	$t=180$
No. 1	51.54	47.76	43.96	38.55	33.71	29.31	29.01
No. 2	51.54	47.94	44.09	39.19	34.12	29.72	29.31
No. 3	51.54	47.38	43.51	38.39	34.2	29.88	29.70
ΔP_1	0.02	−0.57	−0.83	−0.27	0.42	0.47	0.57
ΔP_1	0.02	−0.75	−0.96	−0.91	0.01	0.06	0.27
ΔP_1	0.02	−0.19	−0.38	−0.11	−0.07	−0.1	−0.12
P_z (atm)	51.56	47.19	43.13	38.28	34.13	29.78	29.58

7. Conclusions

We can conclude from the analysis of the calculated values of the average reservoir pressure that the smallest deviation of the numerical results from the measured values is received using the third linearization method. Comparing the values in the tables, no improvement of the results for methods 1 and 2 by reduction of the time step was obtained. The numerical experiments performed for a real object and the measured input data show the high efficiency of the approaches offered in the article in numerical modeling of mass transport through a porous medium of a complex structure.

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