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Calculation of colloids filtration in a porous medium

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Abstract. Construction of underground storage facilities for hazardous radioactive waste requires soil grouting to prevent the penetration of groundwater. Modern technologies of grouting use a liquid-type colloidal silica grout which is injected in a porous soil and forms a protective waterproof layer after solidification. Colloids filtration in a porous medium is an important problem of underground hydromechanics.
The purpose of the study is the numerical solution of the filtration problem of suspensions and colloids in a porous medium. A fluid with fine particles is injected into an empty porous medium. Suspended particles are transported by the fluid flow in a porous medium and partially get stuck in the pores. Calculation of the suspended and retained particles concentrations, depending on time and coordinate, is the theoretical basis of the soil grouting technology.
The one-dimensional problem of deep bed filtration with suspended solid particles in a porous medium for variable porosity and permeability is solved by modified finite difference methods. The use of standard methods for solving the problem is impossible because of the solution discontinuity on the mobile boundary of two-phases. To calculate the global solution near the line of discontinuity and away from it, the counter-current scheme, the Lax-Wendroff scheme and the Total Variation Diminishing finite difference scheme are used. To eliminate the effects of dissipation and dispersion in the TVD-scheme various functions-delimiters are used.
The result of this work is the numerical solution of the nonlinear filtration problem in a porous medium with size-exclusion mechanism of particles retention. The curvilinear two-phase boundary is calculated. A comparison of obtained numerical solutions using different methods of constructing difference schemes is provided. The graphs of suspended particles concentrations are constructed in dependence on time and coordinates.
The comparison of the numerical solutions obtained by different finite-difference methods makes it possible to choose the best way for solving the filtration problem. The counter-current scheme strongly smoothes out the solution on the line of fracture. Using a non-monotonic Lax-Wendroff scheme, a solution with unnatural oscillations near the two-phase boundary is obtained. To calculate the filtration problem, TVD-schemes are the most acceptable. The best result is obtained when using the TVD-scheme with the function-delimiter min2.

1. Introduction

Construction of underground radioactive waste storage facilities requires the soil grouting for groundwater protection. A new material - durable liquid-type colloidal silica grout - is used for construction of a waterproof barrier. The grout mortar is injected under pressure into the porous soil. As a result of filtration, the grout fills the pores of the soil and forms a dense layer that stops water flow [1].

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The filtration of suspensions and colloids is the process of particles passage through the pores of a porous medium and the dynamics of retention. In the considered problem at the initial time the liquid with a given initial concentration of retained particles is injected into the inlet of a porous medium sample of length 1 (a filter). A suspension gradually displaces water and fills the porous medium. In the part of the porous medium before the suspended particles concentration front, the suspended particles concentration is zero, the retained particles concentration does not change on time and is equal to the initial one.

The solution of the filtration problem is determined by the solution of the hyperbolic system of equations. For a number of important particular cases, exact [2-4] and asymptotic solutions of the filtration problem [5-9] are obtained, but in the general case the problem has no analytic solution.

The most efficient and economical way to solve this problem numerically is the finite difference method [10]. However, due to discontinuous initial-boundary conditions, there are significant difficulties to obtain the acceptable solutions near the discontinuity line **-** the suspended and retained particles concentrations front.

The purpose of this paper is to transform the Lax-Wendroff difference scheme into a TVD scheme, and to obtain an adequate solution of the filtration problem both in the neighborhood of the discontinuity and far from it.

A mathematical model of grout filtration in a porous medium and its characteristic features are considered in Section 2. The numerical calculation method (TVD-scheme) is given in Section 3. Section 4 is devoted to the calculation of the finite-difference filtration model. The discussion and conclusions finalize the paper in Sections 5 and 6.

2. Mathematical model

In the domain $\Omega = \{0 < x < 1, t > 0\}$ the suspended and retained particles concentrations $C(x,t)$, $S(x,t)$ satisfy equations

$$\frac{\partial\big(g(S)C\big)}{\partial t} + \frac{\partial\big(f(S)C\big)}{\partial x} = -\Lambda(S)C\,, \tag{1}$$

$$\frac{\partial S}{\partial t} = \Lambda(S)C \tag{2}$$

with boundary and initial conditions

$$x = 0: C(x,t) = p,\;\; p > 0, \tag{3}$$

$$t = 0: C(x,t) = 0,\; S(x,t) = S_0(x)\,. \tag{4}$$

Here, the porosity $g(S)$, the permeability $f(S)$, the filtration coefficient $\Lambda(S)$ and initial deposit concentration $S_0(x)$ are continuous positive functions.

Equations (1)-(2) form a nonlinear (quasilinear) hyperbolic system of the first order. The characteristic curve Γ starting from the origin is the two-phase boundary. It divides the domain Ω into two subdomaines Ω_w and Ω_s with water and suspension. (Fig. 1). In the domain Ω_w the suspended particles concentration $C(x,t)$ is zero, the retained particles concentration $S(x,t)$ is independent on the time and is equal to $S_0(x)$. In the domain Ω_s the unknown concentrations $C(x,t)$ and $S(x,t)$ are positive. According to the method of characteristics, because of the inconsistency of conditions (3-4) at the origin, the solution $C(x,t)$ has a strong discontinuity on the boundary Γ. The solution $S(x,t)$ is continuous throughout the whole domain $\Omega = \Omega_w \cup \Omega_s$ and has a derivative discontinuity at the front Γ.

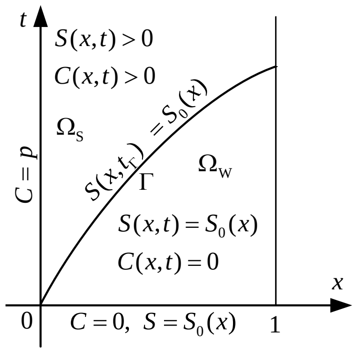

Figure 1. The solution scheme of the problem (1)–(4).

For non-constant functions $g(S)$, $f(S)$ the boundary Γ is a curve determined by the equation

$$t_\Gamma(x) = \int_0^x \frac{g(S_0(u))}{f(S_0(u))}\,\mathrm{d}u\,. \tag{5}$$

For simplification of the system we introduce new functions

$$D(x,t) = g(S)\cdot C(x,t),\ L(S) = \frac{\Lambda(S)}{g(S)},\ m(S) = \frac{f(S)}{g(S)}\,. \tag{6}$$

In the domain $\Omega = \{0 < x < 1,\, t > 0\}$ the functions $D(x,t)$, $S(x,t)$ satisfy the equations

$$\frac{\partial D}{\partial t} + \frac{\partial\big(m(S)D\big)}{\partial x} = -L(S)D\,, \tag{7}$$

$$\frac{\partial S}{\partial t} = L(S)D \tag{8}$$

with boundary and initial conditions

$$x = 0: D = g(S(0,t))\cdot p,\ \ p > 0\,, \tag{9}$$

$$t = 0: D = g(S_0(x))C_0(x),\ S = S_0(x)\,, \tag{10}$$

where $S(0,t)$ can be found from equation (2), which is converted into an ordinary differential equation at $x = 0$

$$\frac{\mathrm{d}S(0,t)}{\Lambda(S(0,t))} = p\,\mathrm{d}t \tag{11}$$

with initial condition $S(0, t = 0) = S_0(0)$.

3. TVD-scheme

We determine a grid in the limited domain $\Omega_{\mathrm{XT}} = \{(x,t)\,|\,0 \le x \le 1,\ 0 \le t \le T\}$

$$x_j = jh,\quad j = 0,1,2,\ \dots,\ J,\quad h = \frac{1}{J};\quad t_n = n\tau,\quad n = 0,1,2,\ \dots,\ N,\quad \tau = \frac{T}{N}, \tag{12}$$

where J is partition intervals number of the segment [0, 1], N is partition intervals number of the segment [0, T], h is the grid step along the filter length x, and τ is a grid step on the time t.

In the filtration problem with zero initial conditions, the concentration front is a straight line. Numerical calculation of such problems can be performed using a standard difference scheme [11, 12].

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For non-zero initial conditions (4), the mobile two-phases boundary is curvilinear (Fig. 1), and the calculation is significantly complicated [13, 14]. In this case, because of the discontinuity of the initial-boundary conditions, the approximation by the finite-difference schemes of the left-hand sides of equations (1) or (7) either leads to dissipation or to dispersion. It leads to dissipation when applying a counter-current scheme with the first order of approximation (the so-called smoothing in the discontinuities points). It leads to dispersion when using a rapidly converging Lax-Wendroff-type schemes with nonphysical oscillations in the discontinuities points (ripples near the discontinuities of the solution).

Varied TVD-schemes (Total Variation Diminishing) - schemes for decreasing the total variation - allow to obtain non-oscillating and appropriate solutions near discontinuities and under certain conditions can provide a high order of convergence in the points of solution continuity [15]. In this case, usually a stable scheme of high order, for example $O(\tau^2+h^2)$, or higher, is modernized by introducing the so-called functions-delimiters, which suppress non-physical oscillations and provide a high rate of convergence of this difference scheme. The resulting modernized difference scheme becomes a scheme preserving the monotony. It means that the scheme pattern transforms a monotonically decreasing or increasing solution from the previous time layer to the next one into a monotone one with decreasing or increasing direction. In this case, a monotone TVD scheme is usually constructed, i.e. a scheme satisfying the nonincreasing condition of the total variation of the solution:

$$TV(D^{n+1}) \le TV(D^n),$$

where

$$TV(D^n) = \sum_{j=0}^{J-1} \left| D_{j+1}^n - D_j^n \right|$$

is the total variation of the grid function [16].

The monotone scheme is constructed only for the first equation of the system (7-10). Equation (8) is solved with the modified Euler method [17].

We write the Lax-Wendroff scheme [18] for equation (7)

$$\frac{\tilde{D}_{j+\frac{1}{2}} - 0.5\left(D_{j+1}^n + D_j^n\right)}{0.5\tau} + \frac{\left(m_{j+1}^n D_{j+1}^n - m_j^n D_j^n\right)}{h} = -L(S_j^n) D_j^n, \tag{13}$$

$$\frac{D_j^{n+1} - D_j^n}{\tau} + \frac{\tilde{m}_{j+\frac{1}{2}} \tilde{D}_{j+\frac{1}{2}} - \tilde{m}_{j-\frac{1}{2}} \tilde{D}_{j-\frac{1}{2}}}{h} = -L(S_j^n) D_j^n \tag{14}$$

and the modified Euler scheme for equation (8)

$$\tilde{S}_j = S_j^n + 0.5\tau L(S_j^n) D_j^n, \tag{15}$$

$$S_j^{n+1} = S_j^n + \tau L(\tilde{S}_j)\tilde{D}_j,\ \tilde{D}_j = 0.5\left(\tilde{D}_{j-\frac{1}{2}} + \tilde{D}_{j+\frac{1}{2}}\right). \tag{16}$$

Due to the fact that the right term of the expression (7) is not equal to zero the approximation accuracy (13)-(14) does not reach $O(\tau^2+h^2)$, but only $O(\tau+h)$.

Expressing $\tilde{D}_{j+\frac{1}{2}}$ and $\tilde{D}_{j-\frac{1}{2}}$ from (13) we obtain

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$$\tilde{D}_{j+\frac{1}{2}} = 0.5\left(D_{j+1}^n + D_j^n\right) - 0.5\tau\left(m_{j+1}^n D_{j+1}^n - m_j^n D_j^n\right)/h - 0.5\tau L(S_j^n) D_j^n . \tag{17}$$

In the right-hand sides of (17) we add and subtract two differences of the type $D_{j+1}^n - D_j^n$. Then, we multiply some new and old terms Φ so that after substituting these expressions in (14), we would be able to isolate a part that coincides with the counter-current difference scheme without, and a separate additional term called the anti-diffusion term. This Φ is called a function-delimiter. We take it with the corresponding index

$$\tilde{D}_{j+\frac{1}{2}} = \frac{1}{2}\left(D_{j+1}^n + D_j^n\right) - \frac{\tau}{2h}\Phi_{j+\frac{1}{2}}\left(m_{j+1}^n D_{j+1}^n - m_j^n D_j^n\right) - \frac{\tau}{2}L(S_j^n)D_j^n + \frac{1}{2}\left(\Phi_{j+\frac{1}{2}}\left(D_{j+1}^n - D_j^n\right) - \left(D_{j+1}^n - D_j^n\right)\right). \tag{18}$$

Substituting (18) into (14) we obtain

$$\begin{aligned}
&\frac{D_j^{n+1} - D_j^n}{\tau} + \frac{\tilde{m}_{j+\frac{1}{2}} D_j^n - \tilde{m}_{j-\frac{1}{2}} D_{j-1}^n}{h} + \frac{1}{2h}\left(\tilde{m}_{j+\frac{1}{2}}\Phi_{j+\frac{1}{2}}\left(\left(D_{j+1}^n - D_j^n\right) - \frac{\tau}{h}\left(m_{j+1}^n D_{j+1}^n - m_j^n D_j^n\right)\right)\right.\\
&\left. -\tilde{m}_{j-\frac{1}{2}}\Phi_{j-\frac{1}{2}}\left(\left(D_j^n - D_{j-1}^n\right) - \frac{\tau}{h}\left(m_j^n D_j^n - m_{j-1}^n D_{j-1}^n\right)\right)\right)\\
&= \frac{\tau}{2h}\tilde{m}_{j+\frac{1}{2}} L(S_j^n)D_j^n - \frac{\tau}{2h}\tilde{m}_{j-\frac{1}{2}} L(S_{j-1}^n)D_{j-1}^n - L(S_j^n)D_j^n ,
\end{aligned} \tag{19}$$

where $\tilde{m}_{j\pm\frac{1}{2}} = m\left(\tilde{S}_{j\pm\frac{1}{2}}\right)$, $\tilde{S}_{j\pm\frac{1}{2}} = \dfrac{\tilde{S}_j + \tilde{S}_{j\pm 1}}{2}$.

When $\Phi \equiv 1$ we return to the Lax-Wendroff scheme with oscillations, but without excessive smoothing in the neighborhood of the discontinuities, and when $\Phi \equiv 0$ we have a counter-current scheme without oscillations, but dissipative in the neighborhood of the discontinuities.

The third term on the left-hand side of (19) can be substantially simplified:

$$\tilde{m}_{j\pm\frac{1}{2}} = m_j^n + O(h),\ m_{j\pm 1}^n = m_j^n + O(h).$$

We obtain

$$\begin{aligned}
&\frac{D_j^{n+1} - D_j^n}{\tau} + m_j^n \frac{D_j^n - D_{j-1}^n}{h} + \frac{m_j^n}{2h}\left(1 - \frac{\tau}{h}m_j^n\right)\left(\Phi_{j+\frac{1}{2}}\left(D_{j+1}^n - D_j^n\right) - \Phi_{j-\frac{1}{2}}\left(D_j^n - D_{j-1}^n\right)\right)\\
&= 0.5\tau m_j^n\left(L(S_j^n)D_j^n - L(S_{j-1}^n)D_{j-1}^n\right)/h - L(S_j^n)D_j^n .
\end{aligned} \tag{20}$$

The left-hand side of (20) is analogous to the linear transport equation and, consequently, three classical functions-delimiters minmod, superbee, Van-Leer can be applied. Despite the rigidity, the scheme (18)-(19) with these limiters operate well for nonlinear systems (1)-(4) or (7)-(10). The third term on the left-hand side of (19) or (20) is the same anti-diffusion term. It eliminates the dissipative term in the first differential approximation of the counter-current scheme, which leads to a decrease in the smoothing effects of the solutions near the discontinuities. At the same time, by reducing the anti-diffusion term, we can reduce the non-physical oscillations on discontinuous solutions.

In addition to our three test functions-delimiters, we apply one more, called min2. But unlike these three functions-delimiters, it does not guarantee high convergence with velocity $O(\tau^2 + h^2)$.

So, we consider a function Φ as a function of a continuous argument ξ, where ξ is determined at the grid nodes $j + \dfrac{1}{2}$

$$\xi_{j+\frac{1}{2}}=\begin{cases}\dfrac{D_j^n-D_{j-1}^n}{D_{j+1}^n-D_j^n} & \text{при} \quad D_{j+1}^n-D_j^n\neq 0;\\ 1 & \text{при} \quad D_{j+1}^n-D_j^n=0.\end{cases} \tag{21}$$

In the case $\xi<0$ (for oscillating solutions) we take $\Phi(\xi)=0$.

The functions-delimiters are

1) minmod $\Phi(\xi)=\max\left(0,\min(1,\xi)\right)$;

2) superbee $\Phi(\xi)=\max\left(0,\min(2\xi,1),\min(2,\xi)\right)$;

3) Van-Leer $\Phi(\xi)=\dfrac{|\xi|+\xi}{|\xi|+1}=\begin{cases}\dfrac{2\xi}{1+\xi} & , \quad \xi>0;\\ 0 & , \quad \xi\leq 0;\end{cases}$

4) min2 $\Phi(\xi)=\max(0,\min(2\xi,2))$.

The plots of these functions are given in Fig. 2.

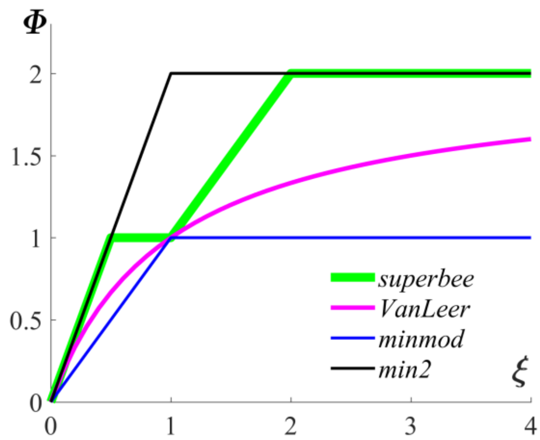

Figure 2. Functions-delimiters.

4. Numerical calculation

The procedure of numerical calculation of the system (7-10) consists of the following steps. First, using formula (21), we find the node values ξ and then the node values of the selected functions-delimiters. Further we find so-called preliminary values $\tilde{S}_j^{n+1}$ (15) and preliminary values $\tilde{D}_{j+\frac{1}{2}}$ from (17). Then we finally obtain the value S_j^{n+1} from (16) and D_j^{n+1} from (19). Substitutions (6) will help to return back from D_j^{n+1} to C_j^{n+1}. For numerical calculation the parameters are chosen: the blocking filtration coefficient $\Lambda(S)=S_{\max}-S$, $S_{\max}=1$, the porosity $g(S)=1+3S$, the permeability $f(S)=1+0.1S$. The initial conditions (4) are $t=0: C=0,\ S=0.5S_{\max}\left(1-x\right)$, $T=4$.

The relationship between step τ in time and step h along the coordinate x is chosen from the Courant convergence

$$\tau\leq\frac{h}{\max\limits_{x\in[0,1],\, t\in[0,T]}\left(m(S(x,t))\right)}. \tag{22}$$

Despite the nonlinearity of equations (1) or (7), this condition can be applied to systems (1)-(4) or (7)-(10), and if this condition is violated, the solution of the systems almost always becomes unstable. For the preliminary calculation τ can be chosen by the formula (22) at $t = 0$.

There is no exact solution to this problem, but for the given initial conditions it is possible to obtain from (5) an exact equation of two-phase boundary Γ:

$$t_\Gamma(x) = 30x + 580\ln\left(1 - \frac{x}{21}\right). \tag{23}$$

The two-phase boundary Γ is presented in Fig. 3. The exact solution (23) is compared with the numerical solution calculated from the counter-current scheme (upwind) and the TVD scheme with the function-delimiter min2 for $J = 10$ and $J = 250$. The boundary Γ is found by integration of formula (5) by left rectangles method after finding the numerical solution of system (7-10).

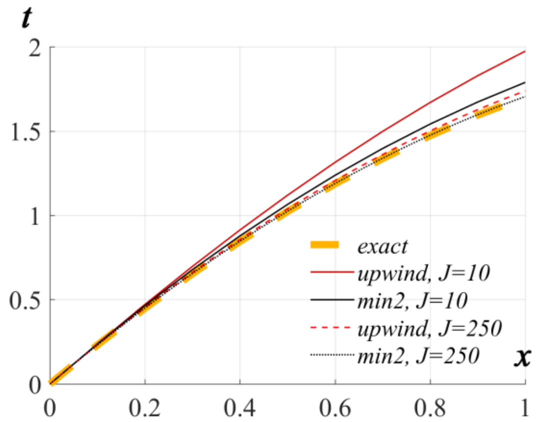

Figure 3. Two-phase boundary Γ.

Fig. 4-7 present the cross sections of the suspended particles concentration $C(x,t)$ in a fixed point $x = 0.5$ for $p = 1$, $J = 200$, $p = 1.2$, $J = 500$, $p = 1.4$, $J = 1000$, $p = 1.6$, $J = 2000$. Each of the figures 4-7 corresponds to the calculation with usage of one of the selected function-delimiter. From the intersection point $t_\Gamma(x)$ and cross sections $x = \text{const}$ or $t = \text{const}$ the vertical perpendiculars (orange solid line) are restored. These lines show the exact places of discontinuities of $C(x,t)$.

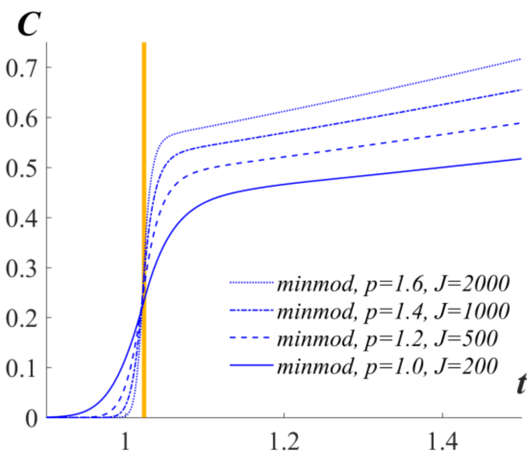

Figure 4. The concentration $C(0.5, t)$ (minmod).

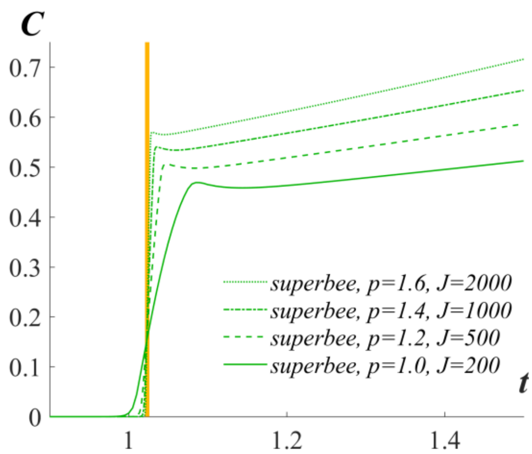

Figure 5. The concentration $C(0.5, t)$ (superbee).

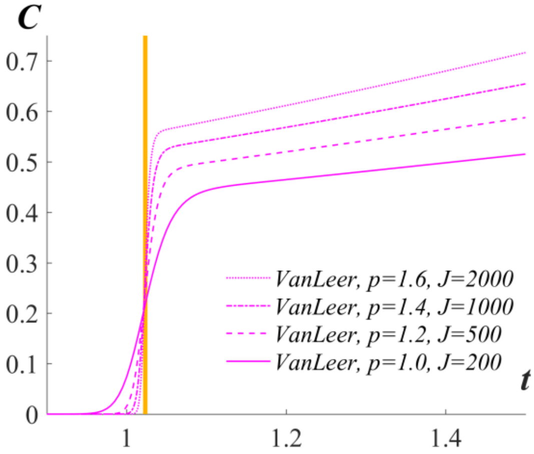

Figure 6. The concentration $C(0.5, t)$ (Van-Leer).

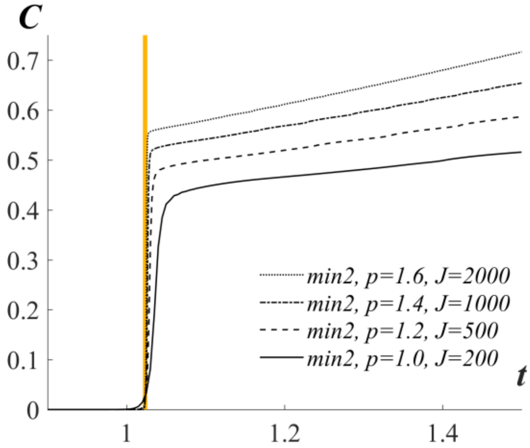

Figure 7. The concentration $C(0.5, t)$ (min2).

Fig. 8, 9 show the cross sections of $C(x,t)$ in a fixed point $x = 0.5$ (Fig. 8) and at the fixed moment of time $t = 0.5$ (Fig. 9) for $p = 1$. The calculation is carried out for counter-current scheme (upwind), Lax-Wendroff scheme (LaxWen) and TVD: minmod, superbee, Van-Leer and min2 for $J = 1000$ and $J = 10000$.

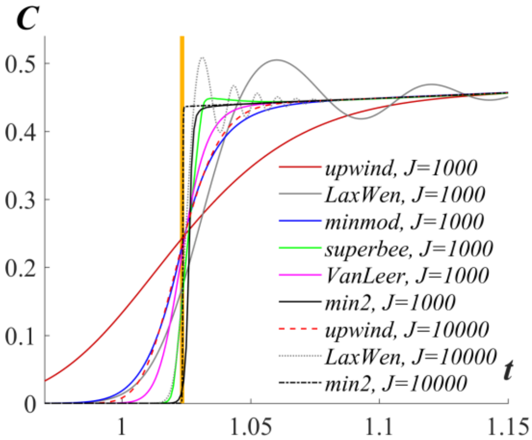

Figure 8. The concentration $C(0.5, t)$.

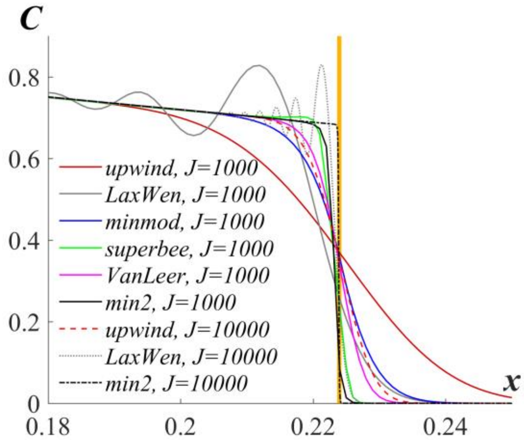

Figure 9. The concentration $C(x, 0.5)$.

5. Discussion

Near the concentration front Γ the counter-current scheme gives a strong smoothing effect of the exact solution, this is the so-called "step" dissipation effect. This effect is eliminated extremely slowly with increasing number of grid points of the finite-difference solution (Fig. 8, 9). A non-monotonic Lax-Wendroff scheme near the place of discontinuity gives unnatural oscillations of the solution, the so-called phenomenon of dispersion. The dispersion area decreases with a thickening of the grid, but it can not be eliminated. As for the TVD-scheme, in comparison with dissipative and dispersive schemes it gives a fairly good result. The calculation of two-phase boundary Γ (Fig. 2) shows that the counter-current scheme converges to the exact solution somewhat worse than one of the TVD-scheme (min2).

Although every function-delimiter was originally obtained for the linear transfer equation, but numerical calculations show that they can be successfully applied to a similar, but nonlinear, filtration equations (1) or (7). However, everything is correct for the given functions of porosity and permeability, as well as for the given initial conditions. The practice of TVD-schemes usage show that function-delimiter superbee is preferable if only initial conditions are changed. Function-delimiter min2 can give oscillations even far from the line of discontinuity. Nevertheless, according to the numerical calculation of this paper, the best result is obtained when using the TVD-scheme with the function-delimiter min2. The function-delimiter superbee converges rapidly near the discontinuity, taking the form of a "step", but we observe an unphysical oscillation (one half-wave) near the discontinuity.

6. Conclusion

A numerical solution of the problem of the suspension flow in a porous medium with using different difference schemes is obtained. The possibilities of using counter-current scheme, non-monotonic Lax-Wendroff scheme, and TVD-scheme with the functions-delimiters for computing the discontinuous solution are studied.

It is shown that solutions obtained when using the counter-current scheme and the Lax- Wendroff scheme have irreparable defects associated with dissipation and dispersion. TVD-schemes are free of these drawbacks. The TVD-scheme with the limiter function-delimiter min2 gives the best approximation of the solution.

The curvilinear mobile two-phase boundary is found numerically and analytically. The cross sections of suspended particles concentration at the fixed moment of time and in a fixed point of a porous media are obtained when using different schemes.

A numerical solution of the mathematical model of grouter filtration in the porous soil allows to prepare a colloidal solution of the optimal composition and to reduce the amount and cost of full-scale experiments [19, 20].

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