Transport through the array of vortices: from microscopic model to macroscopic transport with immobilization

Mikhail R. Khabin¹,², Boris S Maryshev¹,² and Lyudmila S Klimenko¹,²

¹Institute of Continuous Media Mechanics UB RAS, 1 Akad. Koroleva street, 614013 Perm, Russia
²Department of Theoretical Physics, Perm State University, 15 Bukireva street, 614990 Perm, Russia
E-mail: mixail.xabin@mail.ru, bmaryshev@mail.ru, lyudmilaklimenko@gmail.com

Abstract. The paper is devoted to the study of longitudinal solute transport through an array of vortices, bounded by rigid walls. Since the fluid velocity in such system is very heterogeneous, the transfer of solute particles has non-trivial properties. Some particles can flow into the vortex driving by diffusion. These particles do not move in a longitudinal direction. As a result, the observed transport process is similar to the transport with immobilisation. It allows dividing the full solute concentration to mobile and immobile by analogy to the MIM approach. Mobile solute transports with the mean flow in a longitudinal direction. The immobile solute is immobilized by the vortices. The solute transition between these two phases is provided by the diffusion and determined by the concentrations in both phases. The MIM approach is used very often for modelling the transport in porous media. Usually, the particle immobilisation in porous media is explained by the interaction of solute particles with a solid matrix of porous media. However, the flow through porous media is complex and vortices are formed by the interaction of flow with the solid matrix of media. We model the transport of initially heterogeneous distributed solute through the channel by the flow with vortices. The modelling is performed in terms of special flow by the microscopic methods. The distribution of passage time is compared for the same distribution obtained by standard linear macroscopic MIM model. The comparison is performed by the solution of the inverse problem with minimization the difference between these two distributions. As a result, the parameters of the linear MIM model is defined and its dependence on the vortices structure and the molecular diffusivity is obtained.

1. Introduction
One of the most frequently used model of the transport process in a fluid flow is Advection - Diffusion equations (ADE) [1]. Here the Advection is linked to the transportation by the flow itself and the Diffusion describes the random process. These two aspects of transport can be considered independently in the presence of mean macroscopic flow. Wherein, usually, the microstructure of flow is ignored in the description of the advective process. But it is taken into account as macroscopic parameters of the diffusive process. The last method is standard for statistical physics where the random process approach is straightforward than a detailed description of a huge number of microscopic variables. Typical examples in fluid dynamics are turbulence flow [2] and flow through a porous medium [3].
It is known that the transport process through the infinite periodical array of vortices has some features [4]. It is possible to recognize anomalous transport or slow transport process in comparison with ADE model (see [5]). Due to incompressibility of fluid, each vortex contains the trajectory with zero mean velocity. That trajectory, in turn, contains the stagnation point and the fluid element does not move along it (see [4]). The presence of such trajectories slows down the particle transport because the movement near them is very slow. The diffusion can also be the reason for the transport retardation. If the fluid element transits into the vortex by the diffusive process, it becomes immobile. The last effect is not sufficiently examined in the current literature. Also, typical problem consideration for such flows is an infinite unbounded periodical array of such unit cells. This configuration makes the comparison of the microscopic modelling with a macroscopic model more difficult. The aim of the present investigation is a comparison of the effect observed in flows with micro vortices by the statistical method with the results of macroscopic modelling.

The immobilization is often modelled using the MIM (mobile / immobile media) approach [6]. It is assumed that the solute can be divided into two phases. The first is mobile and related to the solute that is moving with the mean flow. The second is immobile and associated with the trapped solute particles. Mathematically, the transport of the mobile solute is modelled by the ADE with the additional term to describe an influx of the solute into the immobile phase. The solute exchange between the phases is described by the additional equation. This equation governs the choice of the specific model which will be used to describe the immobilization process. The simplest model is the linear sorption model or standard MIM model [6, 7]. Where the solute influx between phases linearly depends on concentration in both phases. This model predicts asymmetrical breakthrough curve where the increasing and decreasing of concentration can be fitted by exponential laws with different coefficients. This effect is observed experimentally into the porous media [8] and statistically into the transport through an array of vortices [5].

The paper is organized as follows. Section 1 is devoted to motivation and literature related to the investigated problem. In section 2 the method and problem statement of microscopical modelling the transport through an array of vortices is discussed. The macroscopic problem statement in the framework of linear MIM model and the method of comparison with microscopic modelling is presented in section 3. Section 4 is devoted to discussion about the dependence of macroscopic parameters on microscopic parameter values. The last section 5 is the conclusion where the main results of the present study are summarised.

2. Transportation through array of vortices: microscopic modelling

Let us consider the flow of incompressible fluid inside the square unit cell. The stream function of this flow with non-slip condition on horizontal walls and periodical conditions of vertical wall can be written in form

$$\psi = P \left( \frac{y}{4} - \frac{y^3}{3} + \frac{A}{\pi} \cos(\pi y) \sin(2\pi x) \right),$$

where $A$ is an amplitude of vortex, $y \in [-0.5, 0.5]$ is vertical coordinate and $x \in [-0.5, 0.5]$ is horizontal coordinate. The stream function 1 corresponds to Poiseulle flow with vortex of amplitude $A$. The multiplier $P$ is introduced for manage the mean velocity. It allow us to save the machine time for calculations. The isolines of considered flow is plotted in Figure 1.

The transport of passive particles through this cell is described by the Langevin equations in
The principal streamlines of the flow in unit cell

\[ x_n = \sum_{i=1}^{n} \frac{\partial \psi}{\partial y}(x_{i-1}, y_{i-1}) \tau + \varepsilon \sqrt{2\tau} f_x, \]

\[ y_n = \sum_{i=1}^{n} y_i, \]

\[ y_i = y_k, \quad -0.5 < y_{n-1} + y_k < 0.5, \]

\[ y_i = 1 - 2y_{n-1} - y_k, \quad y_{n-1} + y_k > 0.5, \]

\[ y_i = -1 - 2y_{n-1} - y_k, \quad y_{n-1} + y_k < -0.5, \]

\[ y_k = \varepsilon \sqrt{2\tau} f_y - \frac{\partial \psi}{\partial x}(x_k, y_k) \tau, \]

where \( x_n \) and \( y_n \) are the coordinates of the particle in time \( t_n = \sum_{i=1}^{n} \delta t_i \); \( f_x, f_y \) are independent random variables distributed by normal law (with unit variance and zero mean), \( \varepsilon \) is intensity of diffusion process (\( \varepsilon^2 = D \) where \( D \) is diffusivity) and \( \tau \ll 1/\varepsilon^2 \) is the time step of process, \( x_0 = -0.5 \). The passage time \( T \) is defined numerically as \( T = t_n \) under condition \( x_n \geq 0.5 \). For small values of \( \varepsilon \) the passage time is the function of initial vertical coordinate of the particle \( y_0 \). The passage time is calculated as the mean value of ensemble of 3000 realisations for each value of \( y_0 \). The distributions of passage unit cell time for different intensities \( \varepsilon \) and vortex amplitude \( A \) are shown in Figure 2.

It is seen from Figure 2, the increasing of diffusion intensity leads to decreasing of flow velocity heterogeneity and the enlargement of vortex amplitude leads to intensification transport process.

Using the obtained distribution of unit cell passage time \( T(y) \) it is possible to calculate the passage time for array of \( M \) unit cells in terms of special flow [5]. Due to "stable" [9] property of normal distribution and the incompressibility of fluid, the position of particle at the outer boundary of unit cell (when \( x_n = 0.5 \)) can be defined by the Langevin equation with reflection.
Figure 2. The unit cell passage time $T$ versus initial vertical coordinate of particle $y_0$ at $P = 20$. Left panel: $\varepsilon = 0.05$, curve 1 $A = 0.9$, curve 2 $A = 0.7$, curve 3 $A = 0.3$, curve 4 $A = 0.1$. Right panel: $A = 0.5$, curve 1 $\varepsilon = 0.03$ curve 2 $\varepsilon = 0.07$, curve 3 $\varepsilon = 0.15$, curve 4 $\varepsilon = 0.5$.

of particle from the solid wall of channel

$$y^* = \varepsilon \sqrt{2T(Y_0)f_y - \frac{\partial \psi}{\partial x}(x_k, y_k)T(Y_0)}$$

$$Y_1 = Y_0 + y^*, \quad -0.5 < Y_0 + y^* < 0.5,$$

$$Y_1 = 1 - Y_0 - y^*, \quad Y_0 + y^* > 0.5,$$

$$Y_1 = -1 - Y_0 - y^*, \quad Y_0 + y^* < -0.5.$$  \hspace{1cm} (3)

Eqs 3 can be written in the form $Y_1 = G(Y_0)$. For $M$ cells the transport of single particle is described by the mapping

$$Y_m = G(Y_{m-1}), \quad m = 1..M$$

$$t_M = \sum_{m=0}^{M-1} T(Y_m) \quad \hspace{1cm} (4)$$

The calculation of time $t_M$ of particle passage through array of $M$ unit cells allows to calculate the distribution of passive solute particles passage times for the same array. The concentration for initial heterogeneous distributed particles (at the left boundary on first cell in array) can be calculated as $C(t) = N(t)/N$, where $N$ is the number of particles in the ensemble and $N_t$ is the number of particles with passage times at the interval $t < t_M < t + \delta t$ for $\delta t << t$. The calculated distributions are presented as histograms in Figure 3.

Figure 3 demonstrates standard behaviour for transport with immobilization (see [10]): the dependence of concentration on passage time is highly asymmetrical near inlet and the form becomes more symmetrical after due to the diffusion process.

3. One dimensional transport with immobilization: macroscopic linear MIM model

The transport with immobilization of solute usually modelled by mobile-immobile media (MIM) model (or the two-region solute transport model). Such model is used for investigation of
transport in porous media [11], [12] and describe the experimentally observed slow down of diffusion [13], [10], [14]. Within such a model it is assumed that the solute can be partitioned into distinct mobile (or flowing, with volumic concentration $c$) and immobile (stagnant, with volumic concentration $q$) phases. The solute exchange between these two phases can be modelled by the kinetic equation, which determines the dependence of the solute influx ($\partial_t q$) on the solute concentrations in both phases, or it also can be interpreted as phase transition kinetics. The equations for solute concentration read

$$\partial_t c + \partial_t q = D\nabla^2 c - \mathbf{V} \cdot \nabla c,$$

$$\partial_t q = R(q, c).$$

(5)

where sign $\partial_t$ denotes time derivative, $D$ is effective diffusivity and $\mathbf{V}$ is velocity of carrier fluid. Here the coupling function $R(Q, C)$ can be defined by the specific type of the MIM model.

The simplest and widely used model is the standard or linear MIM model with the following kinetic equation [7]

$$\partial_t q = \alpha (c - K_d q),$$

(6)

where $\alpha$ is the mass transport coefficient and $K_d$ is the solute distribution coefficient [15].

This model provides the correct description of solute transport, especially for low initial concentration, which was confirmed theoretically (for example, [16]) and experimentally [7].

Our aim is comparison our results of microscopic transport modelling with macroscopic model. Because of that, we should solve the one dimensional transport problem in domain $x \in [0, L]$. This problem in terms of Eqs. (5) and (6) can be written as

$$\partial_t C_{tot} = D\partial_x^2 c - V\partial_x c,$$

$$\partial_t q = ac - bq, \quad C_{tot} = c + q$$

$$\partial_x c|_{x=0} = Vc/D, \quad \partial_x C_{tot}|_{x=L} = 0,$$

(7)

where $\partial_x$ derivative with respect of $x$ coordinate, $C_{tot}$ is total solute concentration, $a = \alpha$ is adsorption rate and $b = \alpha K_d$ is desorption rate. Here the last two equations are the boundary conditions, the inlet left boundary is isolated (i.e. no flux of solute at $x = 0$) and at outlet right
boundary is no diffusive flux. The initial conditions are $c|_{t=0} = \Theta(x) - \Theta(x - d)$ $q|_{t=0} = 0$ and where $\Theta(x)$ is Heaviside step function and $d \ll L$. This initial condition is modelled the heterogeneous distribution of solute particles in first unit cell which is used in our microscopic model. The problem (7) is solved numerically by the finite differences method with second order accuracy in space and first order in time. The parameter $d$ from the initial conditions is used as space step of numerical scheme.

The comparison of two models is performed by the solution of inverse problem. It is the problem to obtain the values Eqs. (7) parameters, which provide the minimal value of error function

$$E = \sum_{s=1}^{S} \sum_{k=1}^{K} (C_{tot}(x_s, t_k) - C(x_s, t_k))^2. \tag{8}$$

Here $C_{tot}$ is total concentration, which is calculated form problem (7); $C$ is the concentration which is calculated by the model (4); the $\{x_s, t_k\}$ for $s = 1..S$ and $k = 1..K$ the points in space and time moments where we can calculate the solution by both models. Eqs. (7) contain four parameters, but the mean velocity of carrier fluid can be calculated from the distribution of unit cell passage time as $V = \int_{0.5}^{0.5} 1/T(y)dy$. Note, here the unit of length is the size of unit cell because of the length of domain $L = M$, where $M$ is number of unit cells in modelled array. Another parameters $a$, $b$ and $D$ should be obtained from the solution of inverse problem. The inverse problem is solved by the adjoint state method [17] with using the BFGS algorithm [18] for searching the minimal $E$. The results of this solution and dependences of $a$, $b$ and $D$ on $A$ and $\varepsilon$ is discussed in next section.

4. The identification of macroscopic parameters

The comparison between microscopic and macroscopic model is performed by the second order BFGS method of optimization. The solution of problem should satisfy to the criteria of minimal $E$ value and minimal value of $E$ derivatives with respect of parameters. The derivatives of error $E$ are calculated by the direct adjoin state method. The example of results, which are obtained by both methods, is presented in Figure 4.

It is seen from Figure 4 and the data from the table 1 that the increasing of the vortex intensity $A$ leads to enlargement the effective diffusivity $D$ due to homogenisation of flow velocity (see Figure 2). The dependences of sorption rates $a$ and $b$ on vortex intensity $A$ has a simple explanation. The growth of vortex enhances the immobilisation ability as result the adsorption rate $a$ increases and the desorption rate $b$ decreases. The comparison data for the variation of diffusion process intensity $\varepsilon$ is presented in table 2.

The data which are presented in table 2 show that increasing of diffusion process intensity $\varepsilon$ leads to decreasing of effective diffusivity due to homogenization of fluid velocity profile.

**Table 1.** The microscopic calculation within the framework of (4) are compared to the results of solution the problem (7) for $\varepsilon = 0.05$.

| $A$  | $D$    | $a$      | $b$      | $E$        |
|------|--------|----------|----------|------------|
| 0.1  | 3.01   | $1.35 \times 10^{-2}$ | 3.05 | $9.02 \times 10^{-3}$ |
| 0.3  | 9.70   | $1.64 \times 10^{-1}$ | 2.55 | $7.28 \times 10^{-4}$ |
| 0.5  | $1.33 \times 10^{2}$ | $1.91 \times 10^{-1}$ | 2.41 | $6.04 \times 10^{-4}$ |
| 0.9  | $1.72 \times 10^{2}$ | $2.18 \times 10^{-1}$ | 2.00 | $4.95 \times 10^{-4}$ |
5. Conclusion

The transport of initially heterogeneous distributed solute through the channel by the flow with vortices is modelled into the terms of special flow by the microscopic methods. The distribution of passage time for one unit cell and for an array of identical cells was obtained. The distribution of passage time is compared for the same distribution obtained by standard linear macroscopic MIM model. The comparison is performed by the solution of the inverse problem

Table 2. The microscopic calculation within the framework of (4) are compared to the results of solution the problem (7) for $A = 0.5$.

| $\varepsilon$ | $D$     | $a$       | $b$       | $E$               |
|---------------|---------|-----------|-----------|-------------------|
| 0.03          | $5.74 \times 10^{-2}$ | $7.29 \times 10^{-2}$ | 1.20      | $4.47 \times 10^{-4}$ |
| 0.05          | $1.33 \times 10^{-2}$ | $1.91 \times 10^{-1}$ | 2.41      | $6.04 \times 10^{-4}$ |
| 0.07          | 42.6    | $3.88 \times 10^{-1}$ | 3.62      | $7.17 \times 10^{-4}$ |
| 0.09          | 20.8    | $3.88 \times 10^{-1}$ | 5.91      | $6.02 \times 10^{-4}$ |
with minimization the difference between these two distributions. As a result, the parameters of
the linear MIM model are defined. It is shown that the growth of vortex in the unit cell leads to
increasing the effective diffusivity and immobilising ability. The increasing of diffusion process
intensity leads to homogenisation of flow velocity field and decreasing of effective diffusivity.

Acknowledgments
This work was partially supported by the Grant of the President of Russian Federation (Grant
No. MK-22.2019.1) and by Perm Region Government (Contract C-26/788 from 25.12.2018).

References
[1] Einstein A 1905 Ann. d. Phys. 17 549–60
[2] Frisch U and Kolmogorov A N 1995 Turbulence: The Legacy of A. N. Kolmogorov (Cambridge: University
Press)
[3] Nield D A and Bejan A 2012 Convection in Porous Media (New York USA: Springer-Verlag)
[4] Zaks M A, Pikovsky A S and Kurths J 1996 Phys. Rev. Lett. 77 4338–41
[5] Zaks M A and Nepomnyashchy A 2019 PNAS 116 18245–50
[6] Deans H A 1963 Soc. Petrol. Eng. J. 3 49–52
[7] Van Genuchten M Th and Wierenga P J 1976 Soil Sci. Soc. Am. J. 40 473–80
[8] Bromly M and Hinz C 2004 Water Resour. Res. 40(7)
[9] Levy P and Loeve M 1965 Processus Stochastiques et Mouvement Brownien (Paris: Gauthier-Villars)
[10] Bond W J and Wierenga P J 1990 Water Resour. Res. 26(10) 2475–81
[11] De Smedt F and Wierenga P J 1984 Water Resour. Res. 20 225–32
[12] Wierenga P J and van Genuchten M Th 1989 Ground Water 27 35–42
[13] De Smedt F, Wauters F and Sevilla J 1986 Geoderma 38 223–36
[14] Pachepsky Y, Benson D and Rawls W 2000 Soil Sci. Soc. Am. J. 64 1234–43
[15] Harter R D and Baker D E 1977 Soil Sci. Soc. Am. J. 41 1077–80
[16] Klimenko L S and Maryshev B S 2020 Chem. Eng. J. 381 122644
[17] Fletcher R and Reeves C M 1964 Comput. J. 7(2) 149–54
[18] Nocedal J and Wright S 2006 Numerical Optimization (New York: Springer)