Diffusion effect on passive solute transport inside an infinite two-dimensional array of vortices

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Abstract. The transport process of solute in a two-dimensional liquid flow is studied. The infinite plane is "covered" by square cells with periodic conditions at its boundaries. The flow is provided by a periodic external force. If the amplitude of the external force reaches a certain critical value, then the flow in each cell contains a pair of vortices. The analysis of the transport of a passive solute in such a flow is investigated in terms of a special flow. In the framework of this approach the transport process is described by mapping functions that determine the coordinates of the particle at the end of the unit cell and the time of passage of the cell as a function of the coordinates at the entrance to the cell. These functions are obtained numerically by the random walk method taking diffusion into account. Using the special flow approach the distribution of an initially uniform distributed ensemble of passive particles with time is calculated for the passage of a long array of the unit cells. It is shown that for tiny values of diffusivity the transport slowing down some particles regarding the ensemble is observed. The speed-up of some particles regarding the ensemble is observed for moderate values of diffusivity and for high diffusivity we obtain the standard diffusion.

1. Introduction

During transport of an ensemble of passive particles in complex hydrodynamic flows containing many stagnation points, significant deviations from the classical laws of diffusion can be observed [1]. As it was shown in the work [2], a flow with vortices always contains stagnation points. As the particle trajectory approaches such a point, the time it takes to travel a given distance in the flow, tends to infinity. The logarithmic law of such divergence is established. Also, in the work [3], a study of two-dimensional transport through an array of obstacles in the form of circles was carried out. It is shown that when the trajectory approaches the obstacle, the transit time also tends to infinity, but the divergence is already rooted. In the works [4, 5], the problem was analyzed in the most general form and it was shown that stagnation points with a logarithmic or power-law divergence of the passage time can exist in hydrodynamic flows.

In order to analyze transport through an infinite two-dimensional array of cells, the concept of a special flow was proposed [2]. Within the framework of this concept, there is no need to calculate the coordinates of each particle or to solve equations in the approximation of a continuous medium for the entire array. It
is only necessary to construct a mapping for the coordinates of the exit of a particle from an elementary cell of the array from the coordinates of the entry into it, as well as a function describing the time a particle passes through a given cell. Since the dependence of the travel time of a given distance on the distance to the stagnation point was estimated analytically, in [2-5] idealized functions were used for a special flow, when the stagnation point is placed in the center of the cell and the function is selected that accurately describes the time divergence when approaching it. This approach made it possible to describe the phenomena of sub- and superdiffusion [1-3] for various situations, as well as the phenomenon of particle delay by a stream described in the framework of the standard MIM model [5]. However, an accurate description of particle transport taking into account molecular diffusion within a special flow is impossible, since the mapping function contains a stochastic component that is different for each cell. In papers [4,5], the attempts were made to get around this limitation by introducing some stochastic component directly into the mapping function. It allows showing the transition of anomalous diffusion to normal diffusion and to indicate the scope of applicability of this approach. In this paper, a numerical study of transport in a flow taking into account diffusion is carried out. The mapping functions are obtained numerically, for particles in the flow under random forces by averaging the mapping functions over a large number of iterations, which will allow more correctly taking into account the effect of the random forces on passive particle transport.

2. Liquid flow equations

We consider a two-dimensional flow of a viscous incompressible fluid on an infinite plane with periodic boundary conditions. The governing equations can be written as

\begin{equation}
\frac{\partial \mathbf{V}}{\partial t} + (\mathbf{V} \cdot \nabla) \mathbf{V} = -\frac{\nabla P}{\rho} + \nu \nabla^2 \mathbf{V} + \mathbf{F}(\mathbf{r}, t),
\end{equation}

where \( \mathbf{F} = (f \sin ky, f \sin kx) \) is the external spatially periodic force, \( \mathbf{r} = (x, y) \) are the Cartesian coordinates, \( P \) is the liquid pressure, \( \nu \) is the kinetic viscosity, \( \mathbf{V} = (u, w) \) is the velocity vector, \( l \) is the period of the grid for the considered flow. If the period of the grid is equal to the period of the external force (\( k = 2\pi / l \)), then, according to [4], a solution of Eq. (1) reads

\begin{align}
\begin{aligned}
u &= \alpha - \frac{f}{k^2 \beta^2 + k^2 \nu^2} \cos \left( ky + \arctan \frac{k\nu}{\beta} \right), \\
w &= \beta - \frac{f}{k^2 \alpha^2 + k^2 \nu^2} \cos \left( kx + \arctan \frac{k\nu}{\alpha} \right),
\end{aligned}
\end{align}

where \( f \) is the external force amplitude, \( \alpha \) and \( \beta \) are the mean velocities of the flow in \( x \) and \( y \) directions respectively.

If \( f = 0 \), the solution (2) describes a uniform flow along the direction with an angle with the tangent equals to \( \theta = \beta / \alpha \) (to \( x \) axis). With an increase of the force amplitude \( f \) streamlines start to be bended, and up to \( f = f_c \), when stagnation points are born in the flow [4]. With a further increase in \( f \), each
domain of the flow has a couple of vortices (see [4]). The critical value of the force amplitude can be calculated from the following expression [4]

\[ f_{cr} = k^2 \sqrt{\alpha^2 \beta^2 + k^2 v^2 \max(\alpha^2, \beta^2)}. \] (3)

As it was shown in [2-5], in the case when \( f \geq f_{cr} \) the transport of passive solute particles is of an anomalous nature. Part of the solute is retained by vortices, when the rest of the solute is transported by the flow. The effect of diffusion on such transport has not been investigated in detail.

3. Particle transport equations

The motion of a passive particle with initial position in \((x^0, y^0)\) and suspended in the flow (2) can be described by the following equations

\[
\begin{align*}
x^{i+1} &= x' + u(x', y') \tau + \sqrt{2D \tau} G', \\
y^{i+1} &= y' + w(x', y') \tau + \sqrt{2D \tau} Q'. \\
i' &= i\tau,
\end{align*}
\] (4)

where \( \tau \) is the time step, \( i \) is the step number, \( D \) is the diffusion coefficient, \( G', Q' \) are the independent random variables with Gaussian distribution. Since the domain under study is covered with a lattice consisting of identical cells of the period \( l \), it makes sense to use the approach developed in [5]. In the absence of diffusion, when a particle passes through one cell in a certain direction, its position at the exit from the cell is uniquely described by its initial position. Let us fix the initial \( x \) coordinate for any particle, so let \( x_0 = x^0 = -0.5 \). We consider the passage from \( x_0 \) to \( x_1 = 0.5 \). In this case, the coordinate at the exit \( y_1 = H(y_0 = y^0) \) as well as the passage time for one cell \( t_1 = T(y_0 = y^0) \) are uniquely determined by the flow (2). Thus, the coordinates and passage time for \( n \) cells can be determined as a sum of the corresponding mappings

\[
x_n = n - 0.5, \quad y_n = y_0 + \sum_{j=0}^{n-1} H(y_j), \quad t_n = \sum_{j=0}^{n-1} T(t_j).
\] (5)

This approach has been called the construction of a special flow. The single-valued functions \( H \) and \( T \) exist only in the case when there is no random factor associated with the diffusion. However, if we consider transport through a sufficiently long chain of elementary cells, then it is possible to use a special flow in the form (5), only functions \( H \) and \( T \) should be replaced by their expected values. To obtain the expected values we have calculated the particle motion with floating \( y_0 = y^0 \), and fixed \( x_0 = x^0 = -0.5 \) up to the time moment \( t = t' \), when particle reaches \( x' = 0.5 \). Averaging over the value of the coordinate and time over the set of realizations, we obtain

\[
\begin{align*}
T(y_0) &= \frac{1}{M} \sum_{j=0}^{M-1} t', \\
H(y_0) &= y_1 = \frac{1}{M} \sum_{j=0}^{M-1} y'^j, \\
x'^j = 0.5, \quad x'^{b,j} = -0.5, \quad y'^{b,j} = y^0,
\end{align*}
\] (6)

where \( j \) is the realization number, \( M \) is the full number of random realizations.
The obtained functions \( T(y_0) \) and \( y_1 = H(y_0) \) are presented in Fig.1. It is seen that at small diffusivity \( D \) the dependence \( T(y_0) \) has two peaks which is the sequence of existence of two vortices (see [4]). The increasing of diffusivity leads to homogenization of dependences. The effect of transport slow down for trajectories near stagnation points is reduced.

The mapping in form (5) contains the deterministic functions \( T(y_0) \) and \( y_1 = H(y_0) \), but the description of diffusive process means that we should add also the random displacement and rewrite the mapping (5) in the form

\[
y_j = y_{j-1} + H(y_{j-1}) + \sqrt{2DT(y_{j-1})}G_j,
\]

\[
x_n = n - 0.5, \quad y_n = \sum_{j=0}^{n-1} y_j, \quad t_n = \sum_{j=0}^{n-1} T(y_j).
\]

We study transport of passive tracers through the array of \( n \) cells, neglecting interaction between them. The initial positions of all the \( N \) tracers are randomly chosen from the uniform distribution in the interval \(-0.5 < y_0 < 0.5\). For the passage across the \( n \) cells in \( x \)-direction, each tracer spends the time \( t_p = t_n \). The number of the passive tracers whose passage times range from \( t_p \) to \( t_p + \delta t \), divided by \( N \), can be associated with concentration \( C \), and finally the dependences \( C(t_p) \) for different values of diffusivity can be viewed in Fig. 2—Fig.4.

![Figure 1](image.png)

**Figure 1.** Functions \( T(y_0) \) (left) and \( y_1 = H(y_0) \) (right) obtained for different values of diffusivity, are indicated in the legend. The calculation was performed for \( M = 1000, \ l = 1, \ n = 1, \ \alpha = 1, \ \beta = (\sqrt{5} - 1)/2, \ f = f_0 + 10 = 49.67 \).
Figure 2. The distribution of passage time $c(t_p)$ in linear scale (left) and in semi-logarithmic scale (right) for the array of $n=10^4$ unit cells. The calculation was performed for $D=10^{-3}$, $N=10^4$, $\delta t=0.25$, $M=1000$, $l=1$, $\nu=1$, $\alpha=1$, $\beta=(\sqrt{5}-1)/2$, $f=f_c+10=49.67$. The $t_p=8983$ is the time when the peak of distribution was observed. The red and blue lines indicate the trends for growth and descent tails respectively, the expressions for their time are indicated in the legend.

Figure 3. The distribution of passage time $c(t_p)$ in linear scale (left) and in semi-logarithmic scale (right) for the array of $n=10^4$ unit cells. The calculation was performed for $D=10^{-3}$, $N=10^4$, $\delta t=0.25$, $M=1000$, $l=1$, $\nu=1$, $\alpha=1$, $\beta=(\sqrt{5}-1)/2$, $f=f_c+10=49.67$. The $t_p=8983$ is the time when the peak of distribution was observed. The red and blue lines indicate the trends for growth and descent tails respectively, the expressions for their time are indicated in the legend.
\( l = 1 \), \( \nu = 1 \), \( \alpha = 1 \), \( \beta = (\sqrt{5} - 1)/2 \), \( f = f_{n0} + 10 = 49.67 \). The \( t_c = 9916 \) is the time when the peak of distribution was observed. The red and blue lines indicate the trends for growth and descent tails respectively, the expressions for their time are indicated in the legend.

Figure 4. The distribution of passage time \( C(t_p) \) in linear scale (left) and in semi-logarithmic scale (right) for the array of \( n = 10^4 \) unit cells. The calculation was performed for \( D = 10^{-7} \), \( N = 10^5 \), \( \delta t = 0.25 \), \( M = 1000 \), \( l = 1 \), \( \nu = 1 \), \( \alpha = 1 \), \( \beta = (\sqrt{5} - 1)/2 \), \( f = f_{n0} + 10 = 49.67 \). The \( t_c = 10176 \) is the time when the peak of distribution was observed. The red and blue lines indicate the trends for growth and descent tails respectively, the expressions for their time are indicated in the legend.

As it is shown in Figures 2-3, for small and moderate values of diffusivity the distribution of passage time is asymmetrical. In the case of tiny diffusivity, the concentration growth with time is very fast and after descent of concentration is slower. This effect can be explained by the slowing-down of some particles at the trajectories near the stagnation points or immobilization into vortices. Some particles can enter into the vortex due to diffusion. When the particle is located into the vortex it is excluded from the transport. The exit of a particle from the vortex is also provided by the diffusion. For small diffusivity the enter and exit events are not frequent. The ensemble is moved by the flow with diffusion and some part of particles slows down. As a result, one can observe the distribution which characterizes the transport with immobilization [6]. In the case of moderate diffusivity, the frequency of particle capture by vortex is very frequent and now the moving of the ensemble is slow. Some rare particles are not captured by vortex and they move faster. Here the distribution becomes a non symmetric form with slow growth and fast descent like for transport with speed-up of the particles. The high value of diffusivity leads to the standard transportation process with symmetrical distribution (Figure 4). In this case the diffusive transport dominates over the flow transportation.

4. Conclusion
The study of the transport of passive particles in a vortex flow is carried out taking into account the diffusion process. The approach of a special flow, which makes it possible to significantly simplify the
calculations, is applied. The functions were numerically obtained that specify the mapping of coordinates when a particle passes one domain with a pair of vortices, as well as for the time required for such a passage. Using the obtained functions in the framework of the special flow approach the transport of passive particles ensemble was carried out. The passage time distribution for initially uniform distributed ensemble is calculated for the passage of the array of \( n = 1000 \) unit cells. It is shown that for small values of diffusivity the transport slowing down some particles regarding the ensemble is observed. The speed-up of some particles regarding the ensemble is obtained for moderate values of diffusivity and for high diffusivity the standard diffusion prevails over flow transport.

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