Polymer transport by laminar flows

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Polymer transport is investigated for two paradigmatic laminar flows having open and closed streamlines, respectively. For both types of flows we find transport depletion owing to the action of the polymers elastic degree of freedom. For flows with closed streamlines the leading mechanism for the observed transport reduction is the (dynamical) formation of barriers. For flows with open streamlines the reduction of transport is induced by the renormalization of the bare diffusion coefficient. Results have been obtained by means of Lagrangian simulations.

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The transport of particles advected by a given velocity field is a subject attracting increasing attention of physicists. Such issue has obvious applications in geophysics (e.g. pollutants dispersion) as well as in industrial processes (e.g. transport of a solute in porous media) [1]. In addition, the investigation of the dynamics of particles leads, in a natural way, to highly non trivial behaviors as the anomalous dispersion and the Lagrangian chaos [2,3].

In this paper we investigate the transport of passive polymers in given velocity fields. The interest of this problem is in the spectacular effect of turbulent reduction by the dilute polymer addities (so called drag reduction [4]). Of course, the complete treatment of the drag reduction is very complex and must involve the back-reaction of the polymer concentration on the velocity field ruled by the Navier-Stokes equations [5,6].

A first crude, but non trivial, step is to consider the passive limit, i.e. the transport of polymers in a prescribed velocity field. This problem, in spite of its poor relation with the turbulent drag reduction, is not simple at all. It can be seen as a complication of the, already difficult, issue of the passive particle transport [7].

A widely used model for the polymer dynamics, due to Rouse [8,9], considers macromolecules as a series of $N$ beads linearly connected by harmonic springs. The evolution law is given by the Langevin equations:

$$
\zeta \frac{dR_n}{dt} = -\frac{\partial V}{\partial R_n} + u(R_n) + \eta_n \quad n = 0, \cdots, N-1
$$

where $V = K/2 \sum_{n=1}^{N-1} (R_n - R_{n-1})^2$, $R_n$ is the position of the $n$-th bead, $u$ is the incompressible velocity field, $\zeta$ is the friction coefficient, $K = 3k_BT/b^2$ is the spring constant, $b$ is the average distance between the beads, $k_B$ is the Boltzmann constant, $T$ is the temperature and $\eta_n$ represents the thermal noise mimicking the interaction of beads with the solvent.

The Rouse model (1) can be further simplified (this is the so-called dumbbell model) just taking $N = 2$:

$$
\zeta \frac{dR_0}{dt} = K(R_1 - R_0) + u(R_0) + \eta_0 \quad (2)
$$

$$
\zeta \frac{dR_1}{dt} = K(R_0 - R_1) + u(R_1) + \eta_1. \quad (3)
$$

We assume $\eta_i = \sqrt{2D_0} \tilde{\eta}_i$, with $\tilde{\eta}_i$ normalized, zero-mean, independent white noise processes, and we set, without loss of generality, $\zeta = 1$. For a given velocity field, $D_0$ and $K$ are thus the only relevant parameters controlling the polymer dynamics.

In the following we shall concentrate our attention on the transport properties of the bead center of mass, the coordinates of which are denoted by $R \equiv (R_0 + R_1)/2$, $R \equiv (X,Y)$. Note that in the limit of very large $K$ the evolution equation for $R$ reduces to the usual equation for a fluid particle but with $D_0/2$ instead of $D_0$:

$$
\frac{dR}{dt} = u(R) + \sqrt{D_0} \tilde{\eta}_i. \quad (4)
$$

As in Eqs. (3) and (4), $\tilde{\eta}_i$ is a normalized, zero-mean, white noise process. Therefore, for the understanding of the role of the elastic degree of freedom, results on the diffusion process of the bead center of mass for finite values of $K$ have to be compared with those generated by the particle diffusion limit given by Eq. (4).

The model (4) has been investigated, e.g., in Ref. [11] for a layered random flow, and in Ref. [12] in the presence of a non-potential static random flow. Antithetic conclusions arose for the transport properties of polymers plugged in the two above flow classes. In Ref. [11], the layered random flow has been found to cause an enhanced transport with respect to the single particle diffusion problem. The opposite result (i.e., the occurrence of transport reduction) has been singled out in Ref. [12]. For the flows considered in Ref. [3] the basic mechanism giving rise to transport reduction is played by the dynamically generated barriers, which are not present in the layered random flow [11].
The physical key role for the barrier to emerge is originated from the competition between flow-originated stretching, which acts on the polymers, and the elasticity of the polymeric structure itself. Due to the elastic degree of freedom, unlike particles, polymers have the possibility to select particular regions of the flow. Physically speaking, polymers prefer those regions where they can reduce their own elastic energy. This happens, e.g., in those regions where the velocity strain is large and negative.

The issue related to the possible existence of preferred regions in more realistic flows raised in Ref. \cite{12}. One of the main aim here is to show, by means of numerical simulations, some examples of flows for which transport of polymers is less effective than particles transport. The choice for the flows falls on two paradigmatic laminar velocity fields, the diffusive properties of which have been analyzed in great detail in the past for what concerns particle dispersion \cite{13}. To be specific, we shall focus on shear flows (where the streamlines are open) and cellular flows both stationary and time-dependent (where the streamlines are closed). As we shall see, although for different reasons, such classes of flow show transport depletion in the presence of polymers.

Let us start from the convective flows. We investigate here polymers diffusion in a simple model mimicking the Rayleigh–Bénard convection \cite{14}. Two-dimensional convection with rigid boundary conditions is described here by the following stream function:

$$
\psi(x, y, t) = \psi_0 \sin(x + B \sin \omega t) \sin y, \quad (5)
$$

where the periodicity of the cell is 2\pi, and the even oscillatory instability \cite{14} is accounted for by the term \(B \sin \omega t\), representing the lateral oscillation of the rolls. Velocity is obtained from (5) by the usual relations \(u = (-\partial \psi/\partial y, \partial \psi/\partial x)\). The capability of the simple flow \(\psi\) to capture the essential features of the convection problem is discussed in Ref. \cite{14}.

The second flow we have considered is the two-dimensional Kolmogorov shear flow defined as:

$$
u = (u(y), 0) \quad (6)
$$

with \(u(y) = U \sin(y)\).

Equations (3) and (5) have been integrated with \(u\) obtained from the flows (3) and (5) using a second-order Runge-Kutta scheme. In what follows, averages are extended over different realizations and are performed by following \(\sim 10^5\) couple of particles.

In order to investigate the rate of transport, a measure of the eddy diffusivity, \(D \equiv \langle |X(t) - X(0)|^2 \rangle / (2t)\), for large times, \(t\), has been made, \(X\) being the x-component of the bead center of mass.

Let us start the discussion of our results from the cellular flows. The behavior of the diffusion coefficient, \(D\), vs the spring constant \(K\) are reported in Fig. 1 for \(\omega = 0\) and three different values of the molecular diffusivity. Dashed lines correspond to the particle limit analytically obtained in Ref. \cite{10} (formulae (22) and (24) with \(d = \pi\) and \(\beta = 1\)) in the limit of small \(D_0\).

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig1.png}
\caption{The diffusion coefficient versus the spring constant for the convective model (4) with \(\omega = 0\) and for different values of \(D_0\). Dashed lines represent the theoretical values of the diffusion coefficient obtained in Ref. \cite{10} for the particle diffusion problem.}
\end{figure}

In Fig. 2, the behavior of the average spring elongation, \(l \equiv \langle |R_1 - R_0|^2 \rangle^{1/2}\), is shown as a function of \(K\), again for different values of \(D_0\). Dashed lines correspond to the limit of small \(l\), where it is easily checked that the spring elongations behaves as \((2D_0/K)^{1/2}\).

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig2.png}
\caption{The average spring elongation, \(l\), defined as \(l \equiv \langle |R_1 - R_0|^2 \rangle^{1/2}\), versus the spring constant, for different values of \(D_0\). Dashed lines are relative to the limit of small \(l\), when \(l\) is found to behaves as \((2D_0/K)^{1/2}\).}
\end{figure}
From these figures, a reduction of transport always occurs for spring elongations smaller than the cell size (i.e. $l < \pi$). This is the physically interesting case. The case $l \sim \pi$ corresponds to a minimum in the transport. For small values of $D_0$ (smaller than the smallest one shown in Fig. 1), there exists a narrow band of values of $K$ corresponding to $l \sim \pi$ where particles remain trapped in adjacent cells. The diffusion process stops in this case. Note that this is a pure effect played by the elastic degree of freedom: for the single-particle diffusion in incompressible flows, it is possible to show that the (eddy) diffusion coefficient is always larger than the (bare) coefficient $D_0$.

Transport depletion is here caused by the aforementioned dynamically generated barriers. This can be easily checked in Fig. 4 where the probability density function (pdf) for the bead center of mass to be in the subinterval $[0, \pi] \times [\pi/4, 3\pi/4]$ of the elementary cell is shown for different values of the spring constant $K$ (integration along $y$ has been performed). From this figure it appears as polymers prefer those regions close to the center of the cell where they can reduce their own elastic energy. In such regions, the contribution of the molecular diffusivity to escape from a cell to another is unimportant. On the contrary, the regions close to the cell boundaries, where the role of molecular diffusivity in the (eddy) diffusion process is fundamental, are refused by polymers. The result is the slowing down of the diffusing polymers. Note that the effect of barriers reduces as the spring constant increases. For $K = 0.75$, that corresponds to a spring elongation of $l = 0.40$, the probability density is almost uniform within the cell.

Behaviors similar to those shown in Figs. (1), (2) and (3) have been found also for $\omega \neq 0$. As in Ref. [17], we have restricted our attention only on the case $B = 0.5$.

As one can see in Fig. 3, also in the shear case the diffusion coefficient, $D$, for finite values of $K$ is smaller than that in the limit case of infinite $K$ (see Eq. (3)).

Unlike what happens in the considered cellular flows, this effect is not due to the presence of barriers and can be understood by means of simple arguments. To show that, introducing $\delta y = Y_1 - Y_0$ we immediately have from Eqs. (4), (5) and (6):

$$\frac{d\delta y}{dt} = -2K\delta y + \sqrt{4D_0\tilde{\eta}_1} \quad (7)$$

$$\frac{dX}{dt} = \frac{1}{2}(u(Y - \delta y/2) + u(Y + \delta y/2)) + \sqrt{D_0\tilde{\eta}_2} \simeq u(Y) + \frac{d^2u}{dY^2}\frac{(\delta y)^2}{8} + \sqrt{D_0\tilde{\eta}_2}. \quad (8)$$

Note that in our case $\frac{d\delta y}{dt} = -u$ and, moreover, $\delta y$ performs an Ornstein-Uhlenbeck process, i.e. a Gaussian process with $\langle\delta y\rangle = 0$, $\langle(\delta y)^2\rangle = D_0/K$ and a characteristic relaxation time $\tau = 1/(2K)$. Therefore, from Eq. (8) one sees that the center of mass feels a renormalized velocity field $u(Y) \to u(Y)(1 - \langle(\delta y)^2\rangle/8)$ and a renormalized fluctuation part, i.e. with a larger $D_0$. Now, because of the Taylor formula, $D = D_0/2 + U^2/[2(D_0/2)]$, (note that $D_0 \to D_0/2$ in the particle limit defined by Eq. (3)) it is easy to see that $D$ has negative correction for finite values of $K$.

For a generic time independent shear flow we expect the
same qualitative behavior. This fact can be grasped noting that for $u(y) = \sum_k u_k \exp(iky) + \text{c.c.}$, $u_k$ being the Fourier transform of $u(y)$ and c.c. stands for the complex conjugate, the center of mass experiences a normalized velocity field $\sum_k u_k (1 - k^2/8\langle(\delta y)^2\rangle)$. Exploiting the Zeldovich formula [19], $D \sim \sum_k |u_k|^2/(D_0 k^2)$, in all the realistic cases having rapidly vanishing values of $|u_k|^2$ in the limit $k \to \infty$, the above argument reported for the Kolmogorov flow still holds.

It is worth observing that, for time dependent shear flows, the increasing fluctuating part could give rise to transport enhancement via the interference mechanism identified in Ref. [20]. Indeed, in the presence of anticoerated regions of the velocity field (i.e., where the velocity autocorrelation function is negative), the enhanced molecular diffusivity can be advantageous to escape from the anticoerated regions which slow down the diffusing particle. An enhancement in the diffusion coefficient might occur in this case.

In conclusion, two different mechanisms leading to transport reduction have been identified for two paradigmatic flows with closed and open streamlines, respectively. For stationary flows with closed streamlines transport reduction is due to the emergence of dynamically generated barriers. For stationary flows with open streamlines the mechanism giving rise to the observed reduction of transport is triggered by a renormalized (enhanced) molecular diffusivity. In virtue of such enhanced molecular diffusivity, the bead center of mass forget its past evolution faster than in the case of particles, a fact that reduces the eddy diffusivity. It is an open question whether, in the presence of time-dependent shear flows, the same renormalization of the bare molecular diffusivity might give rise to transport enhancement via the interference mechanism identified in Ref. [20].

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