Asymptotic transport and dispersion of active particles in periodic porous media

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We elucidate the long-time transport of active Brownian particles flowing through a porous lattice using generalized Taylor dispersion theory and Langevin simulations. The asymptotic spreading of a dilute cloud of microswimmers is shown to obey an obstacle-free advection-diffusion equation, which we use to unravel the effects of motility, lattice geometry and fluid flow. Our model suggests that the interplay of particle self-propulsion, entropic trapping by obstacles and shear-induced dispersion can be exploited for controlling the transport of active swimmers through microstructured environments.

The transport of active self-propelled particles through complex microstructured media has important implications in microbial ecology as well as human health. Examples include the spreading of contaminants in soils and groundwater aquifers, bacterial filtering, biodegradation and bioremediation processes, and the transport of motile cells inside the body. Engineering areas such as medical and bioremediation processes, and the transport of motile groundwater aquifers, bacterial filtering, biodegradation
tions in microbial ecology as well as human health. Ex-

we present a macro-continuum transport model based
ple porous matrices remains lacking. In this Letter,
dicting active transport and dispersion in even sim-
models [20–23], yet a general theoretical framework for pre-
ments [11, 17–19] as well as various computational mod-
migration even in quiescent conditions [13–16].

microswimmers along curved boundaries can drive a net
effect similar to upstream swimming in pressure-driven
sensibly leading to a net reduction in mean transport by an
particles in the strong shear near boundaries is expected
induced Taylor dispersion [8, 9]. Secondly, the rotation of

dilute cloud of microswimmers is shown to obey an obstacle-free advection-diffusion equation, which
we use to unravel the effects of motility, lattice geometry and fluid flow. Our model suggests that the
interplay of particle self-propulsion, entropic trapping by obstacles and shear-induced dispersion can
be exploited for controlling the transport of active swimmers through microstructured environments.

Problem definition.— We analyze the long-time asymp-
totic transport of a dilute collection of self-propelled ac-
tive particles dispersed in a viscous solvent and moving
through the interstices of a doubly-periodic 2D porous
material. The porous medium is modeled as an infinite
square lattice comprised of rigid obstacles of character-
istic dimension \(\alpha\) and generated through the discrete
translation of a geometric unit cell of linear dimension \(L\)
(Fig. 1). Each cell in the lattice is labeled by two integers
\((\alpha, \beta) \in \mathbb{Z}^2\), which identify its horizontal and vertical po-
positions \(R_{\alpha\beta} = (X_\alpha, Y_\beta) = L(\alpha, \beta)\) with respect to origin
\(O\), chosen as the centroid of an arbitrary cell. The array
is characterized by its porosity \(\epsilon_p = S_f/S_t\), or ratio of
the interstitial fluid area of a cell over its total area.

In a dilute system, we can neglect interparticle inter-
actions and need only consider the transport of a single
swimmer. Its instantaneous configuration is described by
its position \(R(t)\) with respect to point \(O\) and by its swim-
ning direction \(p = (\cos \theta, \sin \theta)\) in the plane of motion,
where \(\theta(t) \in \Omega = [0, 2\pi]\). The global coordinate \(R\) can be
decomposed as \(R = R_{\alpha\beta} + r\), where \(R_{\alpha\beta}\) is the position
of the unit cell where the particle is located and \(r = (x, y)\)
is a local coordinate with respect to the center of that cell.
The particle is released at \(t = 0\) at position \(R_0 = r_0\) with
orientation \(p_0\). We introduce the following gradient op-

global \(\nabla = \partial/R\), local \(\nabla_r = (\partial/\partial r)R_{\alpha\beta}\) and
orientational \(\nabla_p = (I - pp) \cdot \partial/\partial p\).

Particle motion results from self-propulsion, from ad-
vection and rotation by the fluid flow, and from trans-
lational and rotational diffusion. We model its dynamics
where the initial condition is incorporated by the source terms of local variables as

$$\tilde{R} = v_0 p + u(r) + \eta_i(t),$$  \hspace{1cm} (1)

$$\dot{p} = \frac{1}{2} \Omega(r) \times p + (1 - pp) \cdot \eta_r(t),$$  \hspace{1cm} (2)

where \(\eta_i\) and \(\eta_r\) are Gaussian random vectors with zero mean and variance \(\langle \eta_i(t) \eta_i(t') \rangle = \sqrt{2\kappa} \delta(t - t')\) and \(\langle \eta_r(t) \eta_r(t') \rangle = \sqrt{2\kappa} (1 - pp) \delta(t - t'),\) respectively. The velocity field \(u(r)\) is a 2D Stokes flow driven by a macroscopic pressure gradient applied across the array, with uniform speed \(u_\infty\) and incoming angle \(\Theta_\infty\) upstream of the array; we solve for it numerically by the boundary integral method (see Supplemental Material). The fluid vorticity \(\Omega(r) = \nabla \times u\) also causes rotation of the particle in Eq. (2). Our aim is to describe the long-time fluid vorticity \(\Omega\) (also causing rotation of the array; we solve for it numerically by the boundary integral method). The probability density \(\psi(r, t)\) is the outward unit normal along the cell edges.

\(\psi_0^n\), which describes the long-time probability of finding the particle at local position \(r\) with orientation \(p\) irrespective of which unit cell it is traversing. It satisfies the simplified steady Fokker-Planck equation \(\nabla_r \cdot J_0^n + \nabla_p \cdot j_0^n = 0\), with fluxes

$$J_0^n = [Pc_\infty p + u(r)] \frac{r}{r^2} - \kappa^2 \nabla_r \psi_0^n,$$  \hspace{1cm} (9)

$$j_0^n = \left[ \frac{1}{2} \Omega(r) \times p \right] \frac{r}{r^2} - (1 - pp) \cdot \nabla_p \psi_0^n,$$  \hspace{1cm} (10)

subject to normalization condition \(\int_J \int_0 \psi_0^n \, dp \, dr = 1\), to the no-flux condition \(n_w \cdot J_0^n = 0\) on the surface of the pillar, and to jump conditions \([\psi_0^n] = 0\) and \([\nabla_r \psi_0^n] = 0\) on the unit cell edges \(\partial C_r\) and \(\partial C_t\). We solve for \(\psi_0^n\) numerically using a finite-volume method. \(\psi_0^n\) is then obtained by simple quadrature as

$$\psi_0^n(p, t) = \frac{1}{\Omega} \left[ \psi_0^n(r, p) \right] \left[ U(r) + B(r, p) \right] + O(\epsilon^{-1}).$$  \hspace{1cm} (12)

The fluctuation field \(B(r, p)\) encapsulates information about dispersion and obeys the steady problem

$$\nabla_r \cdot [J_0^n B - \kappa^2 \psi_0^n \nabla_r B] + \nabla_p \cdot [j_0^n B - \psi_0^n \nabla_p B] = -\psi_0^n \bar{U},$$  \hspace{1cm} (13)

subject to the no-flux condition \(n_w \cdot \nabla_r B = 0\) at the obstacle walls, and to jump conditions \([B] = -[r]\) and \([\nabla_r B] = 0\) on \(\partial C_r\) and \(\partial C_t\). We numerically solve for \(B\), and its knowledge provides \(\bar{D}\) as a second quadrature

$$\bar{D} = \frac{1}{2} \int_J \int_0 \left\{ \kappa^2 \psi_0^n \left[ \nabla_r (BB) \right] - J_0^n [BB] \right\} \cdot n \, dp \, dr - \frac{1}{4} \left( \bar{U} B + B \bar{U} \right),$$  \hspace{1cm} (14)
where $\overline{B}$ denotes the spatial and orientational average of $B$ with weighting factor $\psi_0^\infty$.

On long length and time scales, a dilute cloud of active particles is thus expected to be transported with mean velocity $\overline{U}$ and to spread with dispersivity $\overline{D}$ as provided by Eqs. [11] and [14]. This suggests seeking a coarse-grained Eulerian interpretation of $\overline{U}$ and $\overline{D}$ at the so-called Darcy scale, where the fluid and solid obstacles that comprise the porous material become indistinguishable and distances shorter than the characteristic size of the unit cell are irrelevant. To this end, we introduce the discrete conditional probability density

$$\Psi(R_{\alpha\beta}, t; r_0, p_0) = S_t^{-1} \int \int \int \overline{U} \cdot d^2 r d\psi$$

for a particle to be located in cell $(\alpha, \beta)$ at time $t$. On large length scales, we can assimilate $R_{\alpha\beta}$ to a continuous variable $X$ and define a corresponding macro-scale gradient operator $\nabla_X$. The Darcy-scale probability density $\Psi(X, t)$, is then expected to formally satisfy an obstacle-free advection-diffusion equation [25]

$$\partial_t \Psi + \nabla_X \cdot (\overline{U} \Psi - \overline{D} \cdot \nabla_X \Psi) = \delta(X - X_0) \delta(t).$$

As shown below, the analytical solution of Eq. [15] is in exquisite agreement with simulation results at long times, thereby solidifying the interpretation of $\overline{U}$ and $\overline{D}$.

**Results and discussion.**—Results from Brownian Dynamics (BD) simulations of the spreading of a concentrated point source of active swimmers based on Eqs. [1]–[2] are compared to the analytical solution of Eq. [15] in Fig. 2. On short time scales, the cloud develops a complex shape that is continually distorted by the pillars and exhibits wakes, boundary layers, and other features typical of advective-diffusive transport around obstacles. At later times, the cloud shape becomes increasingly smooth and is very well captured by the theoretical model, which predicts spreading into a translating anisotropic Gaussian. This comparison asserts the strength of the Darcy-scale interpretation for describing asymptotic transport, but also highlights key differences. In particular, we observe tailed distributions at pre-asymptotic times in Fig. 2(b), a phenomenon also recently reported in experiments using *E. coli* [11]. The distributions are found to be negatively skewed in the flow direction in strong flows of weakly swimming particles (high $Pe_l$ and low $Pe_s$), whereas they become positively skewed in the opposite case [24]. At longer times, the tails lose their asymmetry and the distributions converge to the asymptotic diffusive solution as shown in Fig. 2(b,c).

Asymptotic transport characteristics can be attributed to pore-scale features of the fluid flow and of the steady-state zeroth-order moment $\psi_0^\infty$ as illustrated in Fig. 2(d). In the absence of flow, the interplay of self-propulsion and translational diffusion near obstacle boundaries creates a net swimmer polarization $\mathbf{m}^\infty(r) = \int \int \psi_0^\infty(r, p) d\mathbf{p}$ against the obstacles [3,5], which vanishes at the cell edges by symmetry. This polarization is accompanied by a net increase in density $\rho_0^\infty(r) = \int \int \psi_0^\infty(r, p) d\mathbf{p}$, which is azimuthally symmetric near a circular obstacle and en-
hanced in regions of high curvature for non-circular pillars [29]. When a flow is applied, the fore-aft symmetry is broken and particles now preferentially accumulate near stagnation points, with a maximum density reached in the rear of circular obstacles. This accumulation, which is observed in experiments [30] and is akin to that occurring at low porosity, dispersion is weak as the pillars act as entropic barriers that hinder active transport [32]. Increasing porosity thus causes a monotonic decrease in $D_{xx}$, as the obstacles act as regions of shear production, thus enhancing shear-induced dispersion. In weaker flows ($Pe_f = 1$), $D_{xx}$ shows a non-monotonic behavior: as porosity is increased, axial dispersion first decreases due to a drop in local shear rate, before increasing again at low obstacle area fractions due to active swimming. Curiously, the limit of $\epsilon_p \to 1$ differs from the case of swimmers in free-space, as infinitesimal obstacles still induce fluid shear in an imposed flow while also modifying the swimmer distribution in their vicinity.

Pillar aspect ratio and fore-aft asymmetry both also affect transport in non-trivial ways. As shown in Fig. 3(c), elliptical obstacles aligned with a weak flow cause higher streamwise dispersion than if aligned perpendicular to it, as the former allow swimmers to glide past while the latter act as entropic barriers that obstruct transport [32]. These trends reverse at high flow rates, as perpendicular obstacles induce stronger velocity gradients thereby enhancing shear-induced dispersion. Fore-aft asymmetric obstacles also lead to complex trends in Fig. 3(d). In the absence of flow, $D_{xx}$ decreases as the shape parameter $Z$ deviates from 0 (circle) by the aforementioned entropic obstruction mechanism. When a flow is applied, fluid shear causes particles to swim along the walls and against the flow, resulting in an enhancement of parti-

FIG. 3. Dispersion in an imposed flow: (a)–(b) Dependence of $D_{xx}$ and $D_{yy}$ on flow Péclet number $Pe_f$ for various values of $Pe_a$, in a lattice with circular pillars for an external flow in the $x$-direction ($\Theta_f = 0$). Inset in (a) highlights strong-flow scalings. (c) Maximum eigenvalue $D_{max}$ of the dispersivity dyadic and (d) corresponding direction of maximum dispersion $\Phi_{D}^{max}$ as a function of incoming flow angle. Parameter values: $Pe_a = 1$, $\kappa^2 = 0.1$, $\epsilon_p = 0.804$. Symbols: BD simulations; lines: analytical model.

Interestingly, activity is seen to hinder $D_{xx}$ in strong flows in Fig. 3(a), as swimming enhances cross-stream migration, which reduces axial spreading within the framework of shear-induced dispersion. Unlike $D_{xx}$, the transverse dispersivity $D_{yy}$ in Fig. 3(b) monotonically decays with $Pe_f$ as stronger flows cause faster rotations of the swimmers in the local shear and thus limit their ability to travel in the $y$-direction.
 FIG. 4. Effect of lattice porosity and obstacle geometry: (a)–(b) Dependence of $\overline{D}_{xx}$ and $\overline{D}_{yy}$ on $p_f$ in the case of circular obstacles at $Pe_s = 1$ and for various flow strengths $Pe_f$. (c)–(d) Effect of shape aspect ratio parameter $\gamma$ and fore-aft asymmetry $Z$ on $\overline{D}_{xx}$ at $Pe_s = 4$ for different values of $Pe_f$. Inset shows obstacle shapes. All plots are for $\Theta_f = 0$ and $\kappa^2 = 0.1$.

conclusion accumulation around obstacles for $Z < 0$ and in a reduction for $Z > 0$. Consequently, the effects of shear alignment (in weak flows) and shear-induced dispersion (in strong flows) on transport are magnified for obstacle shapes that promote accumulation ($Z < 0$), as seen in Fig. 4(c–d). This asymmetry becomes negligible at very high values of $Pe_f$, as activity becomes subdominant and the magnitude of the shear gradients that drive dispersion is independent of the sign of $Z$ by reversibility of Stokes flow.

Concluding remarks.—We have analyzed the long-time transport properties of active particles in a porous lattice under both quiescent and flow conditions. The predictions of our continuum model, which agree perfectly with Langevin simulations at long times, highlight the complex interplay of particle motility, alignment under shear, cross-stream migration, lattice porosity and pillar geometry on asymptotic dispersion. Our theory provides a simple framework for analyzing microorganismal transport in natural structured environments and for designing engineered porous media in applications involving microswimmers. The fundamental premise of non-interacting active Brownian particles glosses over many details that may become relevant in specific systems. Future work should address the roles of hydrodynamic interactions with obstacles 7, swimmer-specific scattering dynamics 13, rheological effects due to activity 14, and the potential emergence of spontaneous flows and active turbulence in denser systems 15.

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