Two-dimensional motion of Brownian swimmers in linear flows

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Abstract The motion of viruses and bacteria and even synthetic microswimmers can be affected by thermal fluctuations and by external flows. In this work, we study the effect of linear external flows and thermal fluctuations on the diffusion of those swimmers modeled as spherical active (self-propelled) particles moving in two dimensions. General formulae for their mean-square displacement under a general linear flow are presented. We also provide, at short and long times, explicit expressions for the mean-square displacement of a swimmer immersed in three canonical flows, namely, solid-body rotation, shear and extensional flows. These expressions can now be used to estimate the effect of external flows on the displacement of Brownian microswimmers. Finally, our theoretical results are validated by using Brownian dynamics simulations.

Keywords Swimming microorganisms · Active Brownian particles · Effective diffusion

1 Introduction

The motion of viruses [1] and bacteria can be affected by thermal fluctuations. Due to their size, these microorganisms may develop a random path (the so-called Brownian motion) due to collisions among molecules forming a fluid and microorganisms [2–8]. These impacts cause the smallest cells to lose their swimming direction [2], which clearly affects their net displacement. An estimate of their net displacement as a function of time may be very valuable in many situations, e.g., in medicine, where to successfully treat and cure infections caused by viruses or bacteria depends on how rapidly we find the patient's disease.

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Moreover, microorganisms are naturally subject to external flows, which is an important factor we should take into account if we wish to have an accurate estimate of their net displacement with time. Examples of external flows acting on viruses and bacteria are, among others, the bloodstream, other flowing corporal fluids, and marine currents affecting the motion of plankton. In addition, the bioengineering community has started to construct microrobots able to propel themselves in a fluid [9–11]. These micromachines are inspired by biomedical applications, e.g., delivering specialized drugs in a more precise region inside our body, or to serve as devices able to detect and diagnose diseases [12–14]. These microrobots, in the same ways as microorganisms, are subject to a very low Reynolds number environment. To mention an example, *E. coli* bacterium, with a typical size of 1–10 μm , swims in water at a speed of around 10 $\mu\text{m/s}$, hence with a Reynolds number of $10^{-5} - 10^{-4}$. In this regime, viscous forces dominate over inertial forces [15], which originates the so-called free net torque and free net force condition on microswimmers, a condition that will be used in the rest of this paper. Due to their size, they will also be subject to thermal fluctuations. This is a very important issue to solve by bioengineers since thermal fluctuations cause the particles to lose their orientation and hence to build a directed robot does not seem a simple task. Other sources of loss of orientation occurring in nature are phase slips [16] and run-and-reverse dynamics [17]. We omit these mechanisms and concentrate on loss of orientation due to rotational Brownian motion. In addition and since the extension to run-and-tumble dynamics [2, 18] is straightforward, we also present an analysis on this mechanism.

Related work concerning passive Brownian particles under external flows, i.e., a spherical Brownian particle under a shear flow [19, 20] and under a general linear flow [21], has already been reported. More recently, active particles (driven by an assumed internal mechanism) have been widely studied [7, 22–29]. For example, the Brownian motion of active bodies of simple shape, one sphere [3, 30], multiple spheres [5], or ellipsoids [30] have been published. Bottom-heavy [31], chemotactic [32] and self-diffusiophoretic [33] active bodies under a shear flow have also been studied. Chemotactic bacteria under a run-and-tumble loss of orientation mechanism and immersed in a shear flow were also reported by Locsei and Pedley [34]. In addition, ten Hagen et al. [35] analyzed, in two dimensions, a spherical active Brownian particle immersed in a shear flow; they found the effect of shear on the diffusion of this particle. We extend that work by studying the effect of any linear incompressible flow on the diffusion of self-propelled particles moving in two dimensions. A three-dimensional study of a spherical swimmer in an incompressible linear flow has also been undertaken [36], and thus our work complements the latter three-dimensional case by considering the motion of active Brownian particles along a plane. This two-dimensional scenario is typical for experimental work, where microswimmers are usually moving over a surface [37] or whose three-dimensional motion is projected onto a plane [3].

In the present paper, we study the motion of natural (microorganisms) and synthetic devices modeled as active (self-propelled) spherical particles swimming in two dimensions, immersed in a general linear flow and subject to thermal forces in translation and rotation. Using a Smoluchowski approach for the rotational degree of freedom, we find the swimmer orientation correlations, which we exploit to calculate the effect of a linear flow on the swimmer diffusivity. Our general theoretical results are applied to three canonical linear flows, namely, solid-body rotation, shear and extensional flows. We observe that the presence of an external linear flow may enhance the effective swimmer diffusion, although it is not always the rule, since it is found that a solid-body rotation flow does not alter the diffusion of an active particle. Superdiffusion is also observed when the particle is immersed in

shear and extensional flows. Finally, our analytical formulas are validated using Brownian simulations.

2 Model

Let us analyze a spherical active (self-propelled) particle of radius a swimming in a two-dimensional fluctuating environment at temperature T and subject to a general linear flow of the form $\mathbf{u}_\infty = (Gx_2, \alpha Gx_1)$ (See Fig. 1). Note that x_1 and x_2 represent Cartesian coordinates while α is a parameter that allows us to change the type of flow where the particle is immersed, i.e., $\alpha = -1$ would correspond to a solid body rotation flow, $\alpha = 0$ to a shear flow, etc. Here G is the deformation rate of the flow. This swimmer is free to rotate along the azimuthal direction φ and its dynamics are described by its translational velocity, $\dot{\mathbf{x}}(t)$ and angular velocity, $\dot{\Omega}(t)$. Here $\mathbf{x}(t)$ is the swimmer position while the dot represents a time derivative. Thermal forces in translation, $\tilde{\mathbf{f}}$, and rotation, $\tilde{\mathbf{g}}$, are modeled as zero-mean random variables whose correlations are given by $\langle \tilde{f}_i(t) \tilde{f}_j(t') \rangle = 2k_B T R_U \delta_{ij} \delta(t - t')$ and $\langle \tilde{g}_i(t) \tilde{g}_j(t') \rangle = 2k_B T R_\Omega \delta_{ij} \delta(t - t')$ according to the fluctuation-dissipation theorem (here $\langle \cdot \rangle$ represents ensemble averaging) [38]. Note that R_U and R_Ω are, respectively, the viscous resistances to translation $R_U = 6\pi\eta a$ and rotation $R_\Omega = 8\pi\eta a^3$, with η the fluid viscosity. Thus, the equation of motion for an active particle swimming at a low Reynolds number and immersed in a linear flow is given by:

$$\dot{\mathbf{x}}(t) = \mathbf{M}\mathbf{x}(t) + U_s(t)\mathbf{e}(t) + \mathbf{f}(t) \quad (1)$$

where we denote by $\mathbf{e}(t)$ the instantaneous unit vector in the direction of swimming with its origin at the center of the particle, $U_s(t)$ is the instantaneous magnitude of the swimming velocity along $\mathbf{e}(t)$ (see Fig. 1 for further details), $\mathbf{f} = R_U^{-1}\tilde{\mathbf{f}}$ and $\mathbf{M}$ is the matrix containing the information from the external flow:

$$\mathbf{M} = \begin{bmatrix} 0 & G \\ \alpha G & 0 \end{bmatrix}. \quad (2)$$

Note that from classical mechanics [39], the dynamics of the orientation vector $\mathbf{e}(t)$ satisfies:

$$\dot{\mathbf{e}}(t) = \dot{\Omega}(t) \times \mathbf{e}(t) \quad (3)$$

Fig. 1 (Color online) Schematics of the studied self-propelled Brownian particle

where $\Omega(t)$ is the swimmer's angular velocity. As already discussed, in a low Reynolds environment, the sphere is subject to the free-torque condition, hence the swimmer's angular velocity for this case is:

$$\Omega(t) = \Omega_\infty + \mathbf{g}(t), \quad (4)$$

where $\mathbf{g} = R_\Omega^{-1} \tilde{\mathbf{g}}$ and $\Omega_\infty = \omega_\alpha \mathbf{k}$ and $\omega_\alpha = G(\alpha - 1)/2$ is the angular velocity induced by the external flow. In our model, the sphere possesses one degree of rotation, namely the angle φ , hence the random torque becomes $\mathbf{g} = g(t)\mathbf{k}$. Thus by explicitly substituting $\Omega(t) = \omega_\alpha \mathbf{k} + g\mathbf{k}$ into (3) and by using the fact that $\mathbf{e}(t) = (\cos \varphi, \sin \varphi)^T$ in the dynamic equation for $\mathbf{e}(t)$, one arrives at a Langevin equation:

$$\dot{\varphi}(t) = \omega_\alpha + g(t), \quad (5)$$

for the rotational degree of freedom. Thus one can easily find the solution to its respective Smoluchowski equation:

$$P(\varphi, t | \varphi_1, t_1) = \frac{1}{\sqrt{4\pi D_\Omega (t - t_1)}} e^{-\frac{(\varphi - \varphi_1 - \omega_\alpha [t - t_1])^2}{4D_\Omega (t - t_1)}}, \quad (6)$$

$$P(\varphi_1, t_1) = \frac{1}{\sqrt{4\pi D_\Omega t_1}} e^{-\frac{(\varphi_1 - \varphi_0 - \omega_\alpha t_1)^2}{4D_\Omega t_1}}, \quad (7)$$

where $P(\varphi, t | \varphi_1, t_1)$ is the conditional probability distribution function (p.d.f.), φ_1 is the angular coordinate at time $t_1 < t$, D_Ω is the rotational diffusion coefficient ($D_\Omega = k_B T / R_\Omega$) and $P(\varphi_1, t_1)$ is the unconditional p.d.f. with an initial condition $\varphi(0) = \varphi_0$. With the knowledge of (6)–(7), the swimmer orientation correlations can be evaluated. They are defined as [40]:

$$\langle e_k(t) e_l(t_1) \rangle = \int d\varphi \int d\varphi_1 e_k(t) e_l(t_1) P(\varphi, t; \varphi_1, t_1) \quad (8)$$

where $P(\varphi, t; \varphi_1, t_1)$ is the joint probability for an orientation φ_1 at time t_1 and φ at time t . This joint probability may be expressed in terms of the conditional probability $P(\varphi, t | \varphi_1, t_1)$ as $P(\varphi, t; \varphi_1, t_1) = P(\varphi, t | \varphi_1, t_1) P(\varphi_1, t_1)$. By directly solving (8), the orientation correlations are finally obtained:

$$\langle e_1(t) e_1(t_1) \rangle = \frac{1}{2} e^{-D_\Omega (t - t_1)} \left[\cos[\omega_\alpha (t - t_1)] + \cos[2\varphi_0 + \omega_\alpha (t + t_1)] e^{-4D_\Omega t_1} \right] \quad (9)$$

$$\langle e_2(t) e_2(t_1) \rangle = \frac{1}{2} e^{-D_\Omega (t - t_1)} \left[\cos[\omega_\alpha (t - t_1)] - \cos[2\varphi_0 + \omega_\alpha (t + t_1)] e^{-4D_\Omega t_1} \right] \quad (10)$$

$$\langle e_1(t) e_2(t_1) \rangle = \frac{1}{2} e^{-D_\Omega (t - t_1)} \left[-\sin[\omega_\alpha (t - t_1)] + \sin[2\varphi_0 + \omega_\alpha (t + t_1)] e^{-4D_\Omega t_1} \right] \quad (11)$$

$$\langle e_2(t) e_l(t_1) \rangle = \frac{1}{2} e^{-D_\Omega (t - t_1)} \left[\sin[\omega_\alpha (t - t_1)] + \sin[2\varphi_0 + \omega_\alpha (t + t_1)] e^{-4D_\Omega t_1} \right] \quad (12)$$

for $t > t_1$. The latter correlations show a classical Brownian exponential decay in orientation [38]. They also indicate that, for long times, the initial condition φ_0 of the swimmer orientation will be irrelevant. These correlations will be needed to explicitly calculate the mean-square displacement tensor $\langle \mathbf{x}(t) \mathbf{x}(t)^T \rangle$. We will perform this calculation in the following section.

3 Mean-square displacement

In order to know the effect of an external linear flow on the net displacement of a microswimmer, we need to find its diffusion tensor $\langle \mathbf{x}\mathbf{x}^T \rangle$. To do so, we first solve (1). By using the definition of the exponential matrix, we are able to integrate (1) and obtain its explicit solution for an initial condition $\mathbf{x}(0) = \mathbf{x}_0$ as:

$$\mathbf{x} = \mathbf{x}_0 e^{\mathbf{M}t} + \int_0^t U_s(t') e^{\mathbf{M}(t-t')} \mathbf{e}(t') dt' + \int_0^t e^{\mathbf{M}(t-t')} \mathbf{f}(t') dt', \quad (13)$$

where one can show that the exponential matrix is given by:

$$e^{\mathbf{M}(t-t')} = \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix} = \begin{bmatrix} \cosh[\sqrt{\alpha}G(t-t')] & \frac{1}{\sqrt{\alpha}} \sinh[\sqrt{\alpha}G(t-t')] \\ \sqrt{\alpha} \sinh[\sqrt{\alpha}G(t-t')] & \cosh[\sqrt{\alpha}G(t-t')] \end{bmatrix}. \quad (14)$$

Note that the deterministic solution to (1) is simply, from (13), $\mathbf{x} = \mathbf{x}_0 e^{\mathbf{M}t}$. We start by calculating the diagonal elements of $\langle \mathbf{x}\mathbf{x}^T \rangle$. In order to simplify the involved expressions, we notice that if $\chi(t)$ corresponds to one component of the particle position, $\chi(t) = x_i(t)$, one can show that:

$$\langle \chi^2(t) \rangle = 2 \int_0^t \left\langle \chi \frac{d\chi}{dt} \right\rangle dt, \quad (15)$$

where we used the initial condition $\chi(0) = 0$. Thus we can combine the components of (1) and (13) and take an ensemble average of the products of those expressions. After some algebra we obtain for the first diagonal element:

$$\begin{aligned} \left\langle x_1 \frac{dx_1}{dt} \right\rangle &= D_B + G \int_0^t U_s(t') b_{1k}(t, t') \int_0^t U_s(t_2) b_{2l}(t, t_2) \langle e_k(t') e_l(t_2) \rangle dt_2 dt' \\ &\quad + G \int_0^t b_{1l}(t, t') \int_0^t b_{2k}(t, t_2) \langle f_l(t') f_k(t_2) \rangle dt_2 dt' \\ &\quad + U_s(t) \int_0^t U_s(t_2) b_{1l}(t, t_2) \langle e_1(t) e_l(t_2) \rangle dt_2 \end{aligned} \quad (16)$$

and for the second diagonal element of the diffusion tensor:

$$\begin{aligned} \left\langle x_2 \frac{dx_2}{dt} \right\rangle &= D_B + \alpha G \int_0^t U_s(t') b_{1k}(t, t') \int_0^t U_s(t_2) b_{2l}(t, t_2) \langle e_k(t') e_l(t_2) \rangle dt_2 dt' \\ &\quad + \alpha G \int_0^t b_{1l}(t, t') \int_0^t b_{2k}(t, t_2) \langle f_l(t') f_k(t_2) \rangle dt_2 dt' \\ &\quad + U_s(t) \int_0^t U_s(t_2) b_{2l}(t, t_2) \langle e_2(t) e_l(t_2) \rangle dt_2 \end{aligned} \quad (17)$$

where we have used the fact that the random force and swimming direction are not correlated, together with the fluctuation-dissipation theorem stating that $\langle f_i(t) f_j(t') \rangle = 2D_B \delta_{ij} \delta(t-t')$, where D_B is the Brownian diffusion constant, $D_B = k_B T / R_U$. Here $k, l \in \{1, 2\}$ following the Einstein summation convention. To calculate the elements out of the diagonal of $\langle \mathbf{x}\mathbf{x}^T \rangle$, we directly use the components of (13). By ensemble averaging the

direct multiplication of these components, together with the fact that the random force and swimming direction are not correlated, leads to the general result:

$$\begin{aligned} \langle x_1(t)x_2(t) \rangle &= \int_0^t U_s(t') b_{1k}(t, t') \int_0^{t'} U_s(t_2) b_{2l}(t, t_2) \langle e_k(t') e_l(t_2) \rangle dt_2 dt' \\ &\quad + \int_0^t b_{1l}(t, t') \int_0^{t'} b_{2k}(t, t_2) \langle f_l(t') f_k(t_2) \rangle dt_2 dt'. \end{aligned} \quad (18)$$

Note that (16)–(18) provide, in a compact notation, the general expression conforming the mean-square displacement tensor for an active particle immersed in any two-dimensional flow of the form $\mathbf{u}_\infty = (Gx_2, \alpha Gx_1)$. Hence these equations generalize ten Hagen's work [35] by considering a general linear flow. Equations (16)–(18) are exactly the same as in [36], however the orientation correlations required in the present work are completely different to those obtained in [36]. In the next section, we apply (16)–(18) to three canonical flows to explicitly see the effect of an external flow on the particle's diffusion moving in two dimensions.

4 Self-propelled particle in three canonical flows

For the sake of simplicity, let us consider a self-propelled particle swimming at constant speed, $U_s(t) = U$, along $\mathbf{e}(t)$, and let us explicitly calculate its effective diffusion when it is immersed in three canonical flows, namely, solid-body rotation flow ($\alpha = -1$), shear flow ($\alpha = 0$), and extensional flow ($\alpha = 1$). Note that (16)–(18) admit in general any time-dependent swimming.

4.1 Solid-body rotation flow

The first case is that of a self-propelled particle swimming at a constant speed, $U_s(t) = U$, along $\mathbf{e}(t)$ and immersed in a solid-body rotation flow ($\alpha = -1$). Solving (16)–(18), together with (15), leads to the following long-time components of its mean-square displacement (MSD):

$$\langle x_1^2(t) \rangle = \langle x_2^2(t) \rangle = \left[2D_B + \frac{U^2}{D_\Omega} \right] t, \quad (19)$$

$$\langle x_1(t)x_2(t) \rangle = 0. \quad (20)$$

In this scenario, the components of the MSD are exactly the same as for the case of an active particle swimming in a quiescent fluid, that is, its MSD for this situation is independent of the surrounding flow. The reason is because the time the particle takes to revolve itself is the same as the time the particle takes to travel along a closed streamline. If it were not the case, the difference in time would generate an extra displacement that would lead to a dependence of the swimmer's diffusion on the surrounding flow. Additionally, solving (16)–(18) together with (15) and applying the limit $t \rightarrow 0$, leads to the following short-time components of its mean-square displacement (MSD):

$$\langle x_1^2(t) \rangle = 2D_B t + U^2 t^2, \quad (21)$$

$$\langle x_2^2(t) \rangle = 2D_B t, \quad (22)$$

$$\langle x_1(t)x_2(t) \rangle = 0. \quad (23)$$

Once again, the MSD components are independent from the surrounding flow.

4.2 Shear flow

The next case is that of a self-propelled particle swimming at a constant speed, U , along $\mathbf{e}(t)$ and immersed in a shear flow. Solving (16)–(18) for $\alpha = 0$, together with (15), leads to the following long-time components of its MSD:

$$\begin{aligned} \langle x_1^2(t) \rangle = & \left[\frac{8}{3} D_B D_\Omega^2 \text{Pe}^2 + \frac{4}{3} U^2 D_\Omega \frac{\text{Pe}^2}{1 + \text{Pe}^2} \right] t^3 + 4U \text{Pe}^2 \left[\frac{\text{Pe}^4 + \text{Pe}^2 - 3}{(1 + \text{Pe}^2)^2 (4 + \text{Pe}^2)} \right] t^2 \\ & + \left[\frac{U^2}{D_\Omega} \frac{(16 + 88\text{Pe}^2 - 19\text{Pe}^4 - 19\text{Pe}^6)}{(4 + 5\text{Pe}^2 + \text{Pe}^4)^2} \right] t + 2D_B t, \end{aligned} \quad (24)$$

$$\langle x_2^2(t) \rangle = \left[2D_B + \frac{U^2}{D_\Omega} \frac{1}{1 + \text{Pe}^2} \right] t, \quad (25)$$

$$\langle x_1(t)x_2(t) \rangle = \left[2D_B D_\Omega \text{Pe} + U^2 \frac{\text{Pe}}{1 + \text{Pe}^2} \right] t^2 + \left[\frac{2U^2}{D_\Omega} \frac{\text{Pe}(\text{Pe}^2 + \text{Pe}^4 - 3)}{(1 + \text{Pe}^2)^2 (4 + \text{Pe}^2)} \right] t. \quad (26)$$

Note that we have introduced the dimensionless Peclet number defined as $\text{Pe} = G/2D_\Omega$, which is the ratio of the orientation decorrelation time and a characteristic time of the flow. The shear flow case was partly reported by [35], where only the leading term of (24) was presented. Here, we provide the whole expressions for all the components of the MSD.

We notice that by setting $\text{Pe} = 0$ in the latter equations, we recover the isotropy of the MSD for an active Brownian particle in a quiescent flow. By substituting $U = 0$ into (24)–(26), we also recover the case of a passive Brownian particle under a shear flow reported in [21], namely:

$$\langle x_1^2(t) \rangle = \frac{2}{3} D_B G^2 t^3 + 2D_B t, \quad (27)$$

$$\langle x_2^2(t) \rangle = 2D_B t, \quad (28)$$

$$\langle x_1(t)x_2(t) \rangle = D_B G t^2. \quad (29)$$

Finally, one can easily show that the leading term of (24) is identical to the reported expression in [35] for the case of an active particle immersed in a shear flow. In a slightly modified ten Hagen notation, his reported dominant term is:

$$\langle \tilde{x}_1^2 \rangle = \frac{32}{9} \xi^2 \left[1 + \frac{3}{8} \frac{\Lambda}{1 + \gamma^2} \right]. \quad (30)$$

If we make the substitutions $\xi = G/2D_\Omega = \text{Pe}$, $\Lambda = (4/3) \beta a F$, $\tilde{x}_1 = x_1/a$, $\gamma = -\xi$, $D_\Omega = (3/4) D_B/a^2$, $\tau = D_\Omega t$ and $U = (4/3) \beta a^2 F D_\Omega$ into (30), we recover the dominant term we have in (24). Note that F represents a force and $\beta = 1/k_B T$ according to ten Hagen nomenclature. Finally, (24)–(26) show that the activity of the particle in a shear flow provides extra coefficients to its MSD that scale in time in the same way as a passive particle under shear. The only difference with the passive case relies on the component $\langle x_1^2(t) \rangle$, where a new quadratic term in time appears due to the activity of the particle.

The short-time components of the mean-square displacement (MSD) can also be found:

$$\langle x_1^2(t) \rangle = 2D_B t + U^2 t^2, \quad (31)$$

$$\langle x_2^2(t) \rangle = 2D_B t, \quad (32)$$

$$\langle x_1(t)x_2(t) \rangle = 2\text{Pe} D_B D_\Omega t^2. \quad (33)$$

Note that the diagonal components of the MSD tensor are independent of the surrounding flow. However, the off-diagonal depends on it.

4.3 Extensional flow

Let us now consider a swimming particle at a constant speed, U , along $\mathbf{e}(t)$ and immersed in an extensional flow. Solving (16)–(18) for $\alpha = 1$ together with (15) leads to the following long-time components of the MSD :

$$\begin{aligned}\langle x_1^2(t) \rangle &= \langle x_2^2(t) \rangle = \langle x_1(t)x_2(t) \rangle \\ &= \frac{D_B}{4\text{Pe}D_\Omega} e^{2Gt} + \frac{U^2}{8D_\Omega^2} \frac{1}{\text{Pe}(1+2\text{Pe})} e^{2Gt}.\end{aligned}\quad (34)$$

In this situation all the components of the mean-square displacement are the same and grow exponentially. It can also be seen that the activity of the particle adds an extra coefficient to its MSD. By setting $U = 0$ and substituting $\text{Pe} = G/2D_\Omega$ into (34), we recover the result obtained by [21]:

$$\langle x_1^2(t) \rangle = \langle x_2^2(t) \rangle = \langle x_1(t)x_2(t) \rangle = \frac{D_B}{2G} e^{2Gt} \quad (35)$$

which shows that all the components of the diffusion tensor for a passive particle also exponentially grow with time. Finally, the short-time components of its mean-square displacement (MSD) are:

$$\langle x_1^2(t) \rangle = 2D_B t + U^2 t^2, \quad (36)$$

$$\langle x_2^2(t) \rangle = 2D_B t, \quad (37)$$

$$\langle x_1(t)x_2(t) \rangle = 4\text{Pe}D_B D_\Omega t^2. \quad (38)$$

5 Brownian dynamics simulations

In order to validate our theoretical results, we compare them with Brownian dynamics simulations. To this end, we consider a spherical swimmer of radius $a = 1 \mu\text{m}$, in water at $T = 300 \text{ K}$ and simulate the motion of this particle swimming at a constant speed ($U_s(t) = U = 1 \mu\text{m/s}$) and immersed in three canonical flows, each of them with a deformation rate of $G = 0.1 \text{ s}^{-1}$ or equivalently $\text{Pe} = 0.313$. Figure 2 shows typical Brownian paths for this swimmer immersed in: a solid-body rotation flow [Fig. 2a]; shear flow [Fig. 2b]; and extensional flow [Fig. 2c] during 100 s. We clearly see that the particle tends to swim along the streamlines of each flow, although the particle can also cross streamlines due to its own internal energy.

To make our comparison quantitative, we plot in Fig. 3 the mean-square displacement of a spherical particle with the same parameters described in Fig. 2 and immersed in a solid-body rotation flow. Its MSD was obtained using 2000 realizations during a period of 1000 s (circles) for the long-time simulation [Fig. 3a] and for 1 second for the short-time simulation [Fig. 3b]. The theoretical results (shown as dashed lines) correspond to (19, 21, 22). Figure 3(a) shows that for $t > 10 \text{ s}$, the theoretical and numerical results start to converge; here the linear behavior of the mean-square displacement with time can be observed. Figure 3 also shows an excellent quantitative agreement between the computational results and our analytical predictions for short and long times. In Fig. 4, we show the MSD of an active particle (same parameters as in Fig. 2) immersed in a shear flow. Its MSD was obtained

Fig. 2 (Color online) Brownian dynamics simulations showing the superposition of seven realizations during 100 s of a spherical swimmer (radius $a = 1 \mu\text{m}$, swimming speed $U = 1 \mu\text{m/s}$, in water at 300 K) immersed in three canonical flows: **a**, solid-body rotation flow; **b**, shear flow with $G = 0.1 \text{ s}^{-1}$ or $\text{Pe} = 0.313$; **c** extensional flow with $G = 0.1 \text{ s}^{-1}$ or $\text{Pe} = 0.313$

with 2000 realizations during a period of 1000 s (circles) [Fig. 4a] and 1 second [Fig. 4b]. The theoretical results (shown as dashed lines) are our (24)–(26) for long times and (31)–(33) for short times. This time, superdiffusion occurs in the long time for $\langle x_1^2(t) \rangle$ and for $\langle x_1(t)x_2(t) \rangle$. An excellent agreement between the computational results and our analytical predictions for short and long times can be observed.

Finally, we plot in Fig. 5 the MSD of the same particle (same parameters as in Fig. 2) but subject to an extensional flow. It can be seen that all the components of its diffusion tensor have the same exponential behavior for long times and in agreement with (34) [Fig. 5a]. Here, the theoretical result given by (34) is shown with square (green) symbols, while the numerical simulations appear in circles. For the short-time dynamics, Fig. 5b shows again an excellent agreement between theory (dashed lines) and simulations.

Fig. 3 (Color online) Brownian dynamics simulations for long and short times, for 2000 realizations during a period of 1000 s (circles) [Fig. 3a] and 1 s (circles) [Fig. 3b] showing the non-zero components of the diffusion tensor of an active particle (same parameters as in Fig. 2) immersed in a solid-body rotation flow. The theoretical results are shown as dashed lines

Fig. 4 (Color online) Brownian dynamics simulations for long and short times, for 2000 realizations during a period of 1000 s (circles) [Fig. 4a] and 1 s (circles) [Fig. 4b] showing the components of the diffusion tensor for an active particle immersed in a shear flow (same parameters as in Fig. 2). The theoretical results are shown as *dashed lines*

6 Applications to biology and synthetic microswimmers

Due to the size of microorganisms [2] and their synthetic counterparts, one can study the effect of natural flows (turbulent flow in oceans, lakes, rivers, flows inside the human body driven by cilia, etc.) on the motion of these swimmers as if they were surrounded by linear flows [41]. For example, in oceanic turbulence, the Kolmogorov scale (which is a measure of the length of the smallest vortices in a flow) is of the order of millimeters [42], which allows us to approximate even a turbulent flow as a linear one.

Fig. 5 (Color online) Brownian dynamics simulations for long and short times, for 2000 realizations during a period of 1000 s (circles) [Fig. 3a] and 1 s (circles) [Fig. 3b] showing the components of the diffusion tensor for an active particle immersed in an extensional flow (same parameters as in Fig. 2). The theoretical results are shown as *dashed lines*

Table 1 Typical deformation rates in nature and their corresponding Peclet number, $Pe = G/2D_\Omega$, for a rotational diffusion $D_\Omega = 0.16 \text{ s}^{-1}$

	$G \text{ (s}^{-1}\text{)}$	Pe
Oceanic turbulence	$0.005 - 1.5$ [43]	$0.06\text{--}4.7$
Blood vessels	10^2 [44]	312.5
Capillaries	10^4 [45]	3125

Let us now provide some typical values of the parameters G , Pe , D_B and D_Ω encountered in nature. It has been reported that in the ocean, the typical rate of deformation G is between 0.005 s^{-1} to 1.5 s^{-1} [43]. If one considers a swimmer of length $1 \text{ }\mu\text{m}$, in water at $T = 300 \text{ K}$, one obtains that its translational diffusivity constant is $0.22 \text{ }\mu\text{m}^2/\text{s}$, whereas its rotational diffusivity constant is 0.16 s^{-1} which leads to a Peclet number, $Pe = G/2D_\Omega$, between 0.06 to 4.7. We summarize the latter results in Table 1 and we also present some typical values for G and Pe for two more biological environments, namely, microorganisms in blood vessels and capillaries.

6.1 Spatial effects

Many experimental works dealing with natural and synthetic swimmers have concluded that a two-dimensional (2D) description of their experiments is very reasonable. For example, Ebbens et al. [37] performed experimental measures of a synthetic active particle. They joined two polystyrene spheres and covered them with platinum patches positioned on each bead at different angles. These patches reacted in peroxide fuel and water, thus imparting translation and rotation to the doublets. Since the doublets settled on the bottom of their container, their motion was described following a two-dimensional Langevin approach. They even showed that the asymmetry of the doublets was not relevant from an hydrodynamic point of view. In this sense, our theoretical results may be validated by simply adding external flows to those Janus particles. On the other hand, Howse et al. [3] studied the Brownian motion of a platinum-coated particle propelled by a chemical reaction. They analyzed the 2D projection of the three-dimensional motion for that particle, hence another situation where our results could be relevant. We now turn to discuss the spatial effects on the diffusion of microswimmers subject to linear external flows. By using results provided in [36], together with results from the present work, one can calculate, for each flow, the ratios of the leading terms (long-time limit) for the active part of the MSD tensor in two (2D) and three dimensions (3D). These ratios are summarized in Table 2. It can be seen that the spatial effects cause the components of the diffusion tensor in 2D and 3D to only differ by a multiplicative constant. It can also be seen that if external flows are absent ($G = 0$), the ratios in Table 2 reduce to the numerical value of three. Note that the passive components of the MSD tensor, for all the canonical flows studied, coincide in 2D and 3D, since for the passive case there is not a preferred direction.

Table 2 Ratios of the leading terms for the active part of the MSD tensor in two (2D) and three dimensions (3D)

	Rotation ($\alpha = -1$)	Shear ($\alpha = 0$)	Extension ($\alpha = 1$)
$\frac{\langle x_1^2 \rangle_{2D}}{\langle x_1^2 \rangle_{3D}}$	3	$\frac{3(16D_\Omega^2 + G^2)}{4(4D_\Omega^2 + G^2)}$	$\frac{3(2D_\Omega + G)}{2(D_\Omega + G)}$
$\frac{\langle x_2^2 \rangle_{2D}}{\langle x_2^2 \rangle_{3D}}$		$\frac{3(16D_\Omega^2 + G^2)}{4(4D_\Omega^2 + G^2)}$	$\frac{3(2D_\Omega + G)}{2(D_\Omega + G)}$
$\frac{\langle x_1 x_2 \rangle_{2D}}{\langle x_1 x_2 \rangle_{3D}}$	N/A	$\frac{3(16D_\Omega^2 + G^2)}{4(4D_\Omega^2 + G^2)}$	$\frac{3(2D_\Omega + G)}{2(D_\Omega + G)}$

Table 3 Typical values for the tumbling rate λ , persistence parameter β , swimming speed U and Reynolds number Re , for some real microorganisms based on a microorganism's length of $1 \mu\text{m}$

	$\lambda \text{ (s}^{-1}\text{)}$	β	$U \text{ (}\mu\text{m/s)}$	$Re \text{ (in water)}$
<i>Escherichia coli</i> , Ref. [46]	1	0.33	10	10^{-5}
<i>Chlamydomonas</i> , Ref. [16]	0.091	Unknown	100	10^{-4}
<i>V. alginolyticus</i> , Ref. [46]	3.3	-1	45	10^{-4}

6.2 Run-and-tumble dynamics

Many microorganisms perform a type of motion that consists of swimming along a straight line for a given time (run stage) and then in drastically changing direction (tumble stage). This type of motion is called run-and-tumble dynamics and has been well characterized [2]. If we denote the mean angular change during tumbling events by φ , the persistence parameter by $\beta = \cos\varphi$ and λ as the tumbling rate, the effective enhanced diffusion for an active swimmer moving in two dimensions and performing run-and-tumble dynamics is $D = U^2/(\lambda[1 - \beta])$ [46] (here U stands for the swimming velocity). On the other hand, the enhanced effective diffusion of a swimmer losing its orientation by purely rotational diffusion is $D = U^2/2D_\Omega$. From the latter enhanced diffusivities, the effective rate of decorrelation due to run-and-tumble dynamics and rotational diffusion is simply the sum of the decorrelation rates for each process since we are dealing with independent stochastic processes, thus we should have an effective diffusion coefficient of the form $D = U^2/(\lambda[1 - \beta] + D_\Omega)$. This coefficient provides an effective rotational diffusion coefficient of the form:

$$\bar{D}_\Omega = D_\Omega + \lambda[1 - \beta]. \quad (39)$$

Thus, one can simply substitute $\bar{D}_\Omega$ instead of D_Ω into the analytical results obtained in Section 4 to obtain equations for the MSD of an active swimmer decorrelating in orientation with both rotational diffusion and run-and-tumble dynamics. Given that we extended our findings to run-and-tumble dynamics, we provide in Table 3 some typical values for the tumbling rate λ , the persistence parameter β , swimming speeds U and Reynolds number Re , for some real microorganisms.

7 Concluding remarks

In this paper we theoretically characterized the effective two-dimensional diffusivity of a spherical active particle subject to a general external linear flow, thermal agitation and run-and-tumble dynamics. By using a Smoluchowski approach for the swimmer's rotational Brownian motion, we were able to find by hand the swimmer's orientation correlations. With these correlations, general formulae for the effective diffusivity of a spherical swimmer immersed in a general linear flow were also obtained. The general formulae allowed us to derive explicit expressions (long and short time) for the diffusion tensor of a swimmer immersed in three canonical flows (solid body rotation, shear and extensional flow). These equations revealed that a solid body rotation flow does not affect the particle's effective diffusion, whereas a particle immersed in a shear flow develops superdiffusion, since its MSD components behave in the long time as $\langle x_1^2 \rangle \sim t^3$, $\langle x_2^2 \rangle \sim t$ and $\langle x_1 x_2 \rangle \sim t^2$. An extensional flow also originates a superdiffusive behavior; for this case all the components of the swimmer's effective diffusion tensor exponentially grow in time. We also showed that our

new analytical expressions for the swimmer's diffusion exactly reduce to previous results. Our theoretical formulas can now be used to estimate the effect of external flows on Brownian active particles moving in two dimensions. To validate our theoretical results we also performed Brownian dynamics simulations that showed excellent agreement between theory and numerical experiments for short and long times. Finally, this paper generalizes the work of [35] by providing, in a compact way, expressions for the whole components of the mean-square displacement tensor of an active Brownian particle immersed in a general linear flow. This work also complements our study in three dimensions [36].

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