

Boundary accumulation of active rods in microchannels with elliptical cross-section

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Many motile microorganisms and biomimetic microparticles have been successfully modeled as active rods—elongated bodies capable of self-propulsion. A hallmark of active rod dynamics under confinement is their tendency to accumulate at the walls. Unlike passive particles, which typically sediment and cease their motion at the wall, accumulated active rods continue to move along the wall, reorient, and may even escape from it. In addition to boundary accumulation, active rods also exhibit upstream swimming and a tendency to concentrate in regions of high boundary curvature. The dynamics of active rods at the wall and those away from it result in complex and nontrivial distributions. In this work, we examine how wall curvature and extruding fluid flow affect the distribution of active rods by studying elliptical perturbations of tubelike three-dimensional microchannels, that is, cylindrical confinements with circular cross-sections that are common in both natural systems and practical applications. We develop a computational model for individual active rods and, through both analytical methods and Monte Carlo simulations, investigate how their accumulation distribution depends on the background flow, rotational diffusion, and the cross-sectional aspect ratio. Additionally, we examined the role of wall torque on accumulated active rods. While it promotes escape by aligning rods tangentially along flat walls, we showed, both theoretically and numerically, that stable entrapment can occur at regions of high curvature despite this torque.

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I. INTRODUCTION

Systems of motile agents capable of persistent directed motion fall under the category of active matter. At microscale, such systems can be exemplified by both biological systems, like suspensions of motile bacteria [1], and biomimetic ones, such as those containing chemically driven bimetallic particles [2–4]. Active matter displays many fascinating phenomena related to collective behavior such as large-scale fluid dynamics and flocking [5–8]. The challenge in studying such systems is that they are in fact nonequilibrium by their continuous injection of energy into the system through self-propelled motion of autonomous components [9,10]. This injection of energy can lead to counter-intuitive results such as decreased viscosity [11–14], movement against the background flow [15–22], and the formation of whirls and jets [23–25]. Also, fascinating is the multiscale natural and universal properties of active matter ranging from nanoscale to human-scale [8]. All these emergent non-Newtonian

macroscopic behaviors have intrigued researchers for some time and inspired the development of novel mathematical models to study the underlying behavior. For a complete overview of the field of active matter we recommend consulting a few recent review articles [1,8,10,26].

While the field of active matter is vast and covers many scales, herein, we narrow our focus to the study of self-propelled “active” rods in confined environments. An active rod, a finite directed segment experiencing a constant propulsion force in the direction its facing, has proven to be an efficient model for elongated microswimmers that are constituents of an active matter system [9,27,28]. Distinguishing features of active swimming at confinement, successfully captured by the active rod model, are *bordertaxis*, which is the tendency of active swimmers to accumulate at boundaries, and *negative rheotaxis*, which refers to upstream swimming in the presence of an imposed flow. Furthermore, active Brownian particles, whether they interact or not, tend to concentrate at points of high boundary curvature [29–32].

The wall accumulation can result from different factors such as hydrodynamic attraction by the wall [33] or electrostatic interactions [21]. However, the primary reason for the rod’s accumulation is its activity. In other words, an active rod confined between boundaries, in the absence of mechanisms to avoid them (such as wall repulsion), will inevitably collide with the boundaries over time. Bordertaxis does not require a background flow, and the accumulation of active rods can be observed in an ambient environment. In contrast,

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negative rheotaxis describes how an active rod responds to a background flow. Briefly, negative rheotaxis is caused by the background flow reorienting active rods upstream as they approach a wall. This occurs because of the no-slip boundary conditions: the background flow vanishes at the wall and increases as one moves away from it. Consequently, the drag force exerted by the background flow on the front of the active rod is lower than that on the rear, resulting in a torque that reorients the active rod to face the current, thereby exhibiting negative rheotaxis. Combination of these two phenomena have been mathematically analyzed for simple boundary geometries, for example, in Refs. [27,28] for nozzles and Ref. [34] for a chamber.

There is a rich array of dynamics displayed by active rods near walls that is still not well understood. After colliding with a boundary, accumulated active rods do not simply settle but instead follow the boundary and may even escape from it. Thus, active rod dynamics is a nontrivial combination of swimming in the fluid bulk and on the boundary surface. The geometry of the boundary wall can significantly affect the active rod distribution and properties of their individual trajectories. The most ubiquitous geometries in applications are long cylindrical microchannels with circular or rectangular cross-sectional geometry. It is well known, for example, that bacteria in microchannels with rectangular cross-sections tend to accumulate in the corners, forming a characteristic “four-lane” transport pattern [15,35,36]. Similarly, regions of high boundary curvature act as natural trapping sites, as the confinement geometry at these points restricts particle escape angles and increases residence time near the wall [29–32,37,38]. It is natural to hypothesize that corners and locations of high or low curvature may serve to control the transport of microswimmers such as bacteria, sperms, and biomimetic particles. For example, such a control would be relevant in addressing issues of bacterial contamination due to their upstream swimming, the reason of catheter-associated urinary tract infection, one of the most common type acquired in health care facilities [39], and formation of hazardous bacteria films in channel geometries [40]. Our work is further motivated by a recent experimental finding how bacteria can utilize the upstream swimming near corners and crevices to invade and contaminate microchannels, the effect called “super-contamination” [41]. The term comes from the idea that bacteria could migrate upstream back to a source and thus contaminating it. Though it seems counter-intuitive that bacteria have the ability to have a net progress upstream given the run-and-tumble dynamics of bacteria, mathematical modeling can be used to reveal the underlying dynamics behind these observations.

In this work, we seek to study the effect of cross-sectional geometry on the distributions of active rods extruded inside a three-dimensional (3D) microchannel and statistical properties of their individual trajectories. Our focus is on how the distribution of an individual active rod depends on the boundary curvature in a three-dimensional microchannel under a background flow. To this end, we consider an elliptical cross-section, so that the curvature varies along the cross-section. Furthermore, we illuminate the effect of key parameters such as the flow rate, rotational diffusion, and aspect ratio of the cross-section in the channels on the macroscopic behavior

of active rod distribution and the effect that varying curvature has on the distribution. We use the mathematical model developed herein to investigate through histograms of active rod distributions in the cross-section. This investigation lays the groundwork for further theoretical and experimental approaches toward complete understanding of geometric control of bacterial contamination.

II. METHOD

We generalize the model from Ref. [27] to study the dynamics of active, rod-shaped swimmers in a cylindrical microchannel with various cross-sectional shapes, subjected to background Poiseuille flow. The three main components of the model, detailed further below, are the dynamics of the active rod in the fluid, the fluid flow vector field, and the dynamics of the active rod at the microchannel wall. To isolate the main features of active rod extrusion through cylindrical microchannels, we introduce two key simplifying assumptions. First, we focus on the statistical properties of individual active rods, neglecting interactions between them. As a result, our findings are directly applicable to dilute suspensions of elongated active swimmers. While swimming in small groups or densely packed populations may give rise to rich emergent phenomena under cylindrical confinement, such behaviors lie beyond the scope of this work. Second, we assume that interactions between the wall and the active rod are purely mechanical, governed by volume exclusion. This leads to a reaction force exerted by the wall on the active rod. To avoid the no-collision paradox [42,43], the model omits hydrodynamic interactions, thereby allowing rods to make physical contact with the wall.

The state of an active rod is uniquely determined by its center location $\mathbf{r}(t) = (x(t), y(t), z(t))^T$ and the unit orientation vector

$$\mathbf{p}(t) = \begin{bmatrix} \cos(\varphi(t)) \sin(\theta(t)) \\ \sin(\varphi(t)) \sin(\theta(t)) \\ \cos(\theta(t)) \end{bmatrix}. \quad (1)$$

The orientation vector $\mathbf{p}$ defines the rod’s front direction with orientation angles $0 \leq \theta \leq \pi$ and $-\pi \leq \varphi < \pi$, see Fig. 1.

The dynamics of the active rod is calculated from force and torque balances. Namely, assume that the fluid exerts the force $-\eta \mathbf{V} ds$ onto element ds of the rod whose relative velocity with respect to the background flow is

$$\mathbf{V}(s) = \frac{d}{dt}[\mathbf{r} + s\mathbf{p}] - \mathbf{u}|_{\mathbf{r}+s\mathbf{p}}. \quad (2)$$

Here, s is the natural parameter of the rod of length ℓ , so $-\ell/2 \leq s \leq \ell/2$ and vector-function $\mathbf{u}(\mathbf{r})$ describes the background flow and solves Stokes equation. Using the smallness of the rod’s length compared to the width of the microchannel, we can approximate the expression for the relative velocity by

$$\mathbf{V}(s) \approx \dot{\mathbf{r}} - \mathbf{u} + s(\dot{\mathbf{p}} - (\nabla \mathbf{u})\mathbf{p}), \quad (3)$$

where $\mathbf{u}$ and $\nabla \mathbf{u}$ are computed at $\mathbf{r}$. Notations $\dot{\mathbf{r}}$ and $\dot{\mathbf{p}}$ stand for time-derivatives of $\mathbf{r}$ and $\mathbf{p}$, respectively. Parameter η represents the viscous drag coefficient.

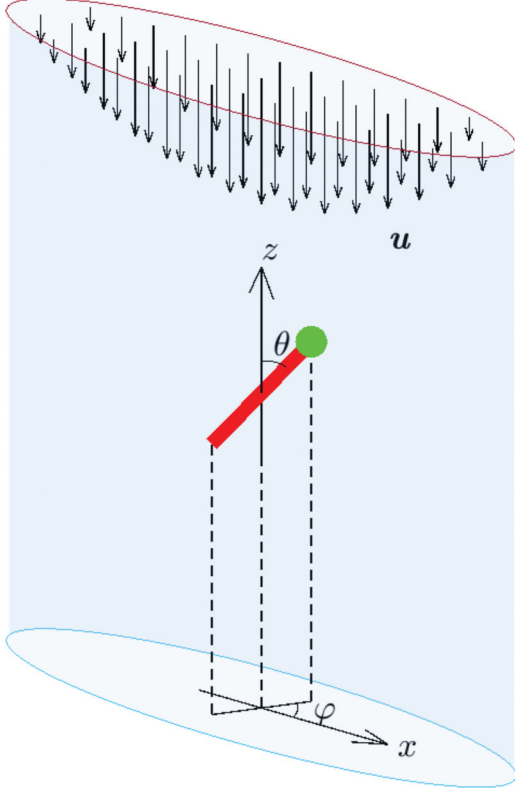


FIG. 1. Illustration for the active rod model. The rod is depicted as a red segment with the green front pointing toward the propulsion direction. Black arrows on the top show fluid flow field $\mathbf{u}$.

The force and torque balances for the active rod are written as

$$\mathbf{0} = -\eta \int_{-\ell/2}^{\ell/2} \mathbf{V}(s) ds + F_{\text{prop}} \mathbf{p}, \quad (4)$$

$$\mathbf{0} = -\eta \int_{-\ell/2}^{\ell/2} s \mathbf{p} \times \mathbf{V}(s) ds + \mathbf{p} \times \sqrt{2D_{\text{rot}}} \dot{\mathbf{W}}. \quad (5)$$

The force balance (4) means that the active rod's movement is determined by the drag force of the background flow on the rod's body [first term in Eq. (4)] and the rod's own propulsion, of strength F_{prop} , in the direction of the rod's orientation $\mathbf{p}$ [second term in Eq. (4)]. The torque balance in Eq. (5) describes how the orientational dynamics of the active rod are governed by the background flow, which induces a torque along the rod's body [first term in Eq. (5)], and by stochastic reorientation, characterized by the rotational diffusion coefficient D_{rot} [second term in Eq. (5)]. The stochastic reorientation term is of the form $\dot{\mathbf{W}} = \dot{W}_{\varphi} \mathbf{e}_{\varphi} + \dot{W}_{\theta} \mathbf{e}_{\theta}$, where

$$\mathbf{e}_{\varphi} = \begin{bmatrix} -\sin(\varphi(t)) \\ \cos(\varphi(t)) \\ 0 \end{bmatrix}, \quad \mathbf{e}_{\theta} = \begin{bmatrix} \cos(\varphi(t)) \cos(\theta(t)) \\ \sin(\varphi(t)) \cos(\theta(t)) \\ -\sin(\theta(t)) \end{bmatrix}.$$

Note that the triple $(\mathbf{p}, \mathbf{e}_{\varphi}, \mathbf{e}_{\theta})$ is an orthonormal basis.

Next, we rewrite Eqs. (4) and (5) as a system for $\mathbf{r}$ and $\mathbf{p}$. To this end, use the expression (3), take the cross product of both sides of Eq. (5) with the vector $\mathbf{p}$, and apply the BAC-CAB

rule implying $\mathbf{p} \times (\mathbf{p} \times \boldsymbol{\tau}) = -\boldsymbol{\tau}$ for $\boldsymbol{\tau} \cdot \mathbf{p} = 0$, and $\mathbf{p} \times (\mathbf{p} \times \mathbf{v}) = -(1 - \mathbf{p}\mathbf{p}^T)\mathbf{v}$ for an arbitrary vector $\mathbf{v}$. We obtain

$$\dot{\mathbf{r}} = \mathbf{u} + v_{\text{prop}} \mathbf{p}, \quad (6a)$$

$$\dot{\mathbf{p}} = (1 - \mathbf{p}\mathbf{p}^T)(\nabla \mathbf{u})\mathbf{p} + \sqrt{2\hat{D}_{\text{rot}}} \dot{\mathbf{W}}, \quad (6b)$$

where $v_{\text{prop}} = (\eta\ell)^{-1}F_{\text{prop}}$ is the propulsion speed and $\hat{D}_{\text{rot}} = 144D_{\text{rot}}/\ell^6\eta^2$ is the effective rotation diffusion coefficient.

It is convenient to rewrite the vector equation (6b) as a system for orientation angles θ and φ . Use the following identity that can be obtained by differentiating Eq. (1):

$$\dot{\mathbf{p}} = \dot{\varphi} \sin(\theta) \mathbf{e}_{\varphi} + \dot{\theta} \mathbf{e}_{\theta}. \quad (7)$$

By using this identity and taking dot products of both sides of Eq. (6b) with $\mathbf{e}_{\varphi}$ and $\mathbf{e}_{\theta}$ we obtain equations for φ and θ , respectively:

$$\begin{aligned} \dot{\theta} &= (\nabla \mathbf{u})\mathbf{p} \cdot \mathbf{e}_{\theta} + \sqrt{2\hat{D}_{\text{rot}}} \dot{W}_{\theta}, \\ \dot{\varphi} &= (\sin(\theta))^{-1} [(\nabla \mathbf{u})\mathbf{p} \cdot \mathbf{e}_{\varphi} + \sqrt{2\hat{D}_{\text{rot}}} \dot{W}_{\varphi}]. \end{aligned} \quad (8)$$

Equations (6a) and (8) describe the active rod's dynamics in the background fluid flow $\mathbf{u}$.

To compute the background flow $\mathbf{u}$ in a fluid of viscosity μ , one needs to solve the incompressible Stokes equation:

$$\begin{aligned} -\mu \Delta \mathbf{u} + \nabla \Pi &= \mathbf{0}, \\ \nabla \cdot \mathbf{u} &= 0, \\ \mathbf{u}|_{\partial M} &= \mathbf{0}. \end{aligned} \quad (9)$$

Here, Π is the pressure and the first two equations hold inside the microchannel M with the boundary wall ∂M . The third equation in Eq. (9) is the no-slip boundary condition at the wall ∂M . The cylindrical geometry of the microchannel allows for simplification of Eq. (9). Namely, let the z axis be the major axis of the cylinder, that is, $M = \{(x, y, z) : (x, y) \in \Omega, -\infty < z < \infty\}$ where Ω is the two-dimensional domain indicating the cross-section geometry. Then Eq. (9) admits a solution in the form $\mathbf{u} = w(x, y)\mathbf{e}_z$ and $\Pi = [\Pi]z$ where $\mathbf{e}_z = (0, 0, 1)$ and $[\Pi]$ is a constant quantifying the pressure gradient along the microchannel. This solution type is relevant for our purposes since it describes a pressure-driven flow along the microchannel. The equation for $w(x, y)$ reduces to a two-dimensional (2D) Poisson's equation with a constant in the right-hand side. Specifically, $w(x, y)$ solves the boundary value problem:

$$\begin{aligned} \Delta_{x,y} w &= [\Pi]/\mu \text{ in } \Omega, \\ w &= 0 \text{ on } \partial\Omega. \end{aligned} \quad (10)$$

This equation has an analytical solution for some geometries Ω such as an ellipse or a rectangle. Background flows $\mathbf{u}$ based on these analytical solutions w are known as Poiseuille flows. For example, if Ω is the ellipse $x^2/a^2 + y^2/b^2 = 1$, then

$$w(x, y) = \frac{a^2 b^2 [\Pi]}{2\mu(a^2 + b^2)} \left[\frac{x^2}{a^2} + \frac{y^2}{b^2} - 1 \right].$$

The constant $[\Pi]/\mu$ is related to the volume v_e of the fluid passing through a given cross-section per unit of time, that is,

$$v_e = \int_{\Omega} |w(x, y)| dx dy = \frac{[\Pi]\kappa}{\mu},$$

where the parameter $\kappa = \int_{\Omega} |\hat{w}(x, y)| dx dy$ depends on geometry of Ω only. Here, $\hat{w}$ is the solution of the boundary-value problem (10) with 1 in place of $[\Pi]/\mu$. For the elliptical cross-section, we have that $\kappa = \int_{\Omega} |\hat{w}| dx dy = \pi a^3 b^3 / (4(a^2 + b^2))$. As it was pointed out in Ref. [27], it is convenient to express the flow rate in terms of the flow speed at the microchannel's center-line $x = y = 0$, which is related to v_e through the following equality:

$$v_e = \frac{\pi ab}{2} |w(0, 0)|. \quad (11)$$

We will introduce the parameter $v_f = |w(0, 0)|$ which can be expressed in terms of v_e by Eq. (11), so that the function w admits a simple form: $w(x, y) = v_f(x^2/a^2 + y^2/b^2 - 1)$.

With the known function $w(x, y)$, we can rewrite the system (8) in a simpler form:

$$\begin{aligned} \dot{\theta} &= -\sin^2(\theta)(w_x \cos \varphi + w_y \sin \varphi) + \sqrt{2\hat{D}_{\text{rot}}} \dot{W}_{\theta}, \\ \dot{\varphi} &= (\sin(\theta))^{-1} \sqrt{2\hat{D}_{\text{rot}}} \dot{W}_{\varphi}. \end{aligned} \quad (12)$$

We formulate boundary conditions for active rods interacting with the confinement boundary. No boundary conditions are imposed in the z -direction, indicating that the microchannel is infinitely long, and the rods are free to move along its length without restriction. We impose that an active rod cannot penetrate the boundary but still can move tangentially along the boundary and reorient. That is, the equation for $\mathbf{r}$ becomes

$$\dot{\mathbf{r}} = (\mathbf{I} - q\mathbf{n}\mathbf{n}^T)(\mathbf{u} + v_{\text{prop}}\mathbf{p}), \quad (13)$$

where $q = 0$ if the rod is in the bulk and $q = 1$ if the rod is at the confinement boundary; vector $\mathbf{n}$ is the unit outward normal vector for Ω . The numerical implementation of this boundary condition is subtle since the rod is never exactly on the wall. It is often the case that when a numerical step is applied to the system (6), the rod's front $\mathbf{r}_f = \mathbf{r} + \ell/2\mathbf{p}$ ends up outside the wall. If this happens, then we adjust the location of the rod $\mathbf{r}$ by shifting it along $-\mathbf{d}\mathbf{n}$ where d is the distance between the front of the rod $\mathbf{r}_f$ and the wall, and $\mathbf{n}$ is the unit of outward normal vector computed at the projection of $\mathbf{r}_f$ onto the wall, $\mathbf{r}_w = (a \cos(\alpha_w), b \sin(\alpha_w), z_f)$. Here, z_f is the z coordinate of $\mathbf{r}_f = (x_f, y_f, z_f)$, and the parameter α_w is the solution of the minimization condition of $\min_{0 \leq \alpha_w < 2\pi} \|\mathbf{r}_f - \mathbf{r}_w(\alpha_w)\|^2$:

$$\begin{aligned} (a^2 - b^2) \cos(\alpha_w) \sin(\alpha_w) - ax_f \sin(\alpha_w) \\ + by_f \cos(\alpha_w) = 0. \end{aligned}$$

After this adjustment, the rod is located inside the computational domain Ω with its front on the wall. We also tested alternative, reasonable implementations of these boundary conditions and found that the model's performance remained consistent across them. One example of such an alternative implementation is to first allow an active rod to swim during the portion of the time step before its front collides with the wall; next, to let the rod swim tangentially along the wall for the remainder of the time step; and finally, to adjust the rod's position so that its front lies exactly on the wall.

We note that the propulsion mechanisms of specific types of microswimmers (e.g., sperm, motile bacteria *Escherichia coli* or *Bacillus subtilis* and bimetallic rods) are highly diverse and complex. In studying the macroscopic properties of active swimmers, such as the dynamics of their distributions, it is

common to represent the propulsion mechanism as a constant force in the direction of $\mathbf{p}$ and do not bother with the details of self-propulsion generation. However, confinement, in addition to being an obstacle, is known to alter the dynamics of microswimmers [44,45], for example, by hydrodynamic attraction or affecting the beating of flagella, a primary means of propulsion for many motile bacteria. Here, our focus is on prototypical active rods that maintain a constant level of self-propulsion away and at the wall, and the wall is merely a geometric constraint expressed by the active rod boundary condition (13). We note that the numerical results in Ref. [28] based on these modeling assumptions showed good agreement with the experiments on bimetallic rods. Generally, any discrepancies between the experimental observations for specific microswimmers and the results of the active rod model described above may highlight the particular features of these microswimmers.

However, we would like to study the effect of the wall torque, which was not considered in earlier works [27,28]. Namely, according to Newton's third law, the active rod experiences a reaction force from the wall that balances its self-propulsion, preventing the active rod penetrating the wall. This force has been taken into account by the term with parameter q in the force balance (13). But this force is applied to the front edge of the active rod and thus introduces a torque that must affect the equation for $\mathbf{p}$. Namely, to take into account this torque we need to add the following term to the right-hand side of the equation (6b):

$$-q\mathcal{T} \frac{6v_{\text{prop}}}{\ell} (\mathbf{n}^T \mathbf{p})(\mathbf{I} - \mathbf{p}\mathbf{p}^T)\mathbf{n}. \quad (14)$$

Here, $\mathbf{n}$ is the outward normal vector where the active rod's front edge $\mathbf{r}_f$ touches the wall. The parameter $\mathcal{T}$ is such that if $\mathcal{T} = 0$, then the wall torque is neglected and if $\mathcal{T} = 1$, then the wall torque is applied. We also can vary $0 \leq \mathcal{T} \leq 1$ to study the role of the wall torque. The derivation of Eq. (14) is relegated to Supplemental Material (SM) [46]. It was shown that the wall torque may help bacteria to escape from wall entrapment [47]. In that study, bacteria are initially passive and attached to the wall. However, after nutrients are added to the suspension, the bacteria become active and start rotating at the wall due to the wall torque, eventually escaping from it.

III. RESULTS

A. Active rods undergoing extrusion in cylindrical microchannels with elliptical cross-sections preserve key features of confined active matter: wall accumulation, negative rheotaxis, and concentrations at regions of highest curvature

Here we consider the case $\mathcal{T} = 0$. To understand how the statistical properties of active rod trajectories change when the ubiquitous geometry of a cylindrical channel with a circular cross-section is perturbed, we consider an elliptical cross-section. That is, we consider the microchannel wall described as $\partial M = \{(x, y, z) | x^2/a^2 + y^2/b^2 = 1\}$, where a and b are semi-major and semi-minor axes, $a > b$.

We begin by examining the case of zero rotational diffusion, which allows for an analytical expression for the distribution of the accumulation of active rods. Note that the background flow field $\mathbf{u}$ has no components in the (x, y) plane.

As a result, the projection of an active rod's trajectory onto the (x, y) plane (i.e., the microchannel cross-section) resembles the motion of a swimmer in a two-dimensional elliptical lake. In this simplified *2D lake problem*, active rods swim in the two-dimensional domain $\Omega = \{x^2/a^2 + y^2/b^2 < 1\}$ with no background flow and rotational diffusion. By contrast, we refer to the original three-dimensional system, with background flow and zero rotational diffusion, as the *3D river problem*. In what follows, we will explore this analogy, highlight the insights it offers for the three-dimensional problem, and a key difference between the two problems.

In the elliptical lake problem, the orientation of the active rod does not change over time, since we disregard all forces that may reorient the rod, such as background shear and rotational diffusion. An active rod will swim straight until it collides with the wall, and then it will slide along the wall until its orientation becomes perpendicular to the wall surface, that is, when the active rod's orientation vector $\mathbf{p}$ coincides with the outward normal vector $\mathbf{n}$. If we simulate many active rods with random initial locations and orientations, then more rods will tend to accumulate at points with the highest curvature. Roughly speaking, this is because vicinities of the highest curvature points have a greater range of direction angles for the outward normal vector compared to vicinities of the same size of points with a lower curvature. To make this statement precise, consider an active rod with the initial orientation $\mathbf{p} = (\cos(\varphi), \sin(\varphi))^T$ so that the orientation angle φ is uniformly random, $\varphi \sim \mathcal{U}(-\pi, \pi)$. Regardless of its initial location, the active rod will converge to the point on the wall where $\mathbf{p} = \mathbf{n}$ (see also SM video 4 [46]). The final location of the active rod can be described by α , the wall parameter so the wall is parameterized as $x = a \cos(\alpha)$, $y = b \sin(\alpha)$ with $-\pi < \alpha \leq \pi$. We show in Supplemental Material [46] that the uniform distributions of the initial orientations φ and the condition for the final location $\mathbf{p} = \mathbf{n}$ imply that the distribution of α is

$$f(\alpha) = \frac{ab}{2\pi(b^2 \cos^2(\alpha) + a^2 \sin^2(\alpha))}. \quad (15)$$

Assuming $a > b$, this probability distribution function $f(\alpha)$ attains its maximum at $\alpha = 0, \pi$, corresponding to the points of the highest curvature, and its minimum at $\alpha = \pm\pi/2$, the lowest curvature points. Note that the form of $f(\alpha)$ in Eq. (15) depends on the choice of the initial distribution for φ . In our analysis, we adopt the uniform distribution for φ as the most representative case. When $\dot{D}_{\text{rot}} > 0$, however, the long-term behavior becomes independent of the initial distribution: $f(\alpha)$ converges to an equilibrium distribution regardless of the initial condition for φ . Below, using numerical simulations, we demonstrate how introducing a perturbation with $D_{\text{rot}} > 0$ modifies the form of $f(\alpha)$. We note that the case with $D_{\text{rot}} > 0$ has also been studied analytically in Ref. [29], under simplifying assumptions that the active agents are modeled as active Brownian particles and the angle between the vectors $\mathbf{p}$ and $\mathbf{n}$ is small. Under these assumptions, the concentration at $\alpha = 0$ and π was obtained.

In the original three-dimensional problem with zero rotational diffusion (the 3D river problem) equations for x and y components of the active rods are of the same type as in the 2D lake problem, and the azimuthal orientation φ is constant. Therefore, it is natural to expect that the (x, y) projection of

an active rod obeys the same dynamics in the (x, y) plane as in the case of the 2D lake problem: the active rod eventually converges to the wall location where the orientation of its cross-sectional projection coincides with the outward normal. The difference is that the velocity in (x, y) plane depends on the polar angle θ and has the speed $v_{\text{prop}} \sin(\theta)$ where θ solves the equation:

$$\dot{\theta} = -v_f \sin^2(\theta) \left(\frac{2x}{a^2} \cos(\varphi) + \frac{2y}{b^2} \sin(\varphi) \right). \quad (16)$$

The polar angle θ converges to either 0 or π , corresponding to orientations parallel to the microchannel's major axis (upstream and downstream, respectively). This reorientation is explained by the effect of background flow shear, which tends to align the active rod with the microchannel. As θ approaches either 0 or π , the velocity in the (x, y) plane vanishes. This raises the following question: *Is it possible that the active rod fails to reach the wall because its orientation converges too rapidly to an alignment parallel to the microchannel?* For instance, one might consider the scenario where $\theta \rightarrow 0^+$ as $t \rightarrow \infty$, and $(x(t), y(t))$ converges to a point strictly inside the domain Ω . In what follows, we show that this is not the case (provided $\sin(\theta) \neq 0$ at the initial time): the active rod does reach the wall in finite time. To this end, we introduce a variable $\rho(t) \geq 0$ such that, while the active rod remains away from the wall, its trajectory in the (x, y) plane is given by $(x(t), y(t)) = (x_0 + \rho(t) \cos(\varphi), y_0 + \rho(t) \sin(\varphi))$, where φ is fixed. Then functions $\theta(t)$ and $\rho(t)$ satisfy the following closed form system of ordinary differential equations:

$$\begin{aligned} \dot{\theta} &= -2v_f \sin^2(\theta)(A + B\rho), \\ \dot{\rho} &= v_{\text{prop}} \sin(\theta), \end{aligned} \quad (17)$$

where $A = (x_0/a^2) \cos(\varphi) + (y_0/b^2) \sin(\varphi)$ and $B = \cos^2(\varphi)/a^2 + \sin^2(\varphi)/b^2$ are constant, and $B > 0$. This system is derived from Eqs. (6a) and (16), and that φ is constant. Note that $0 < \theta(t) < \pi$, and thus $\dot{\rho}(t) > 0$. Therefore, two scenarios are possible: either $\rho(t)$ converges monotonically to a finite value as $t \rightarrow \infty$, or $\rho(t) \rightarrow \infty$. The latter implies that $\rho(t)$ reaches any prescribed positive value in finite time, and hence the active rod reaches the wall in finite time. To rule out the former case, observe that if $\rho(t)$ converges to a finite value, then $\sin(\theta(t)) \rightarrow 0$ as $t \rightarrow \infty$, implying that $\theta(t) \rightarrow 0$ or π . Consider now the following first integral of system (17), i.e., a nonconstant, continuously differentiable function that remains constant along any solution:

$$\frac{1}{B}(A + B\rho(t))^2 + \frac{v_{\text{prop}}}{v_f} \log \left| \tan \left(\frac{\theta(t)}{2} \right) \right| \equiv \text{const.}$$

As $t \rightarrow \infty$, the logarithmic term on the left-hand side diverges, while the remaining terms stay bounded, leading to a contradiction. Thus, $\rho(t) \rightarrow \infty$ as $t \rightarrow \infty$. Furthermore, in the context of system (17), we conclude that $\theta(t) \rightarrow 0$ as $t \rightarrow \infty$, corresponding to the upstream swimming. Indeed, for sufficiently large t , the equation for θ takes the form $\dot{\theta} = -M(t) \sin^2(\theta)$ with $M(t) = 2v_f(A + B\rho) > 1$. Since $\theta(t) \in (0, \pi)$ and $\dot{\theta} \leq -\sin^2(\theta)$, this implies $\theta(t) \rightarrow 0$ as $t \rightarrow \infty$. Thus, we conclude that in the 3D river problem, the active rod

reaches the wall in a finite time and eventually reorients itself against the flow.

However, the time required to reach the wall can be significantly longer than in the 2D lake problem. To illustrate this, take $a = b = R$ (a circular cross-section), and estimate the time for the active rod to swim from $x^2 + y^2 = (R/2)^2$ to $x^2 + y^2 = R^2$ (i.e., the wall). Assume smallness of θ , that $A + BR \propto 1/R$, and that the active rod swims toward the wall with the optimal orientation angle φ , so the initial position is given by: $(x_0, y_0) = \frac{R}{2}(\cos \varphi, \sin \varphi)$. Thus, the first equation in system (17) becomes $\dot{\theta} \approx -\frac{v_f}{R}\theta^2$, whose solution is

$$\theta(t) = \frac{R\theta_0}{\theta_0 v_f t + R}.$$

Integrating the radial velocity equation $\dot{\rho} = v_{\text{prop}}\theta$, we find that the displacement $\rho(t)$ grows logarithmically in time:

$$\rho(t) = \frac{Rv_{\text{prop}}}{v_f} \ln \left(\frac{\theta_0 v_f t}{R} + 1 \right),$$

as opposed to the linear growth $\rho(t) = \rho(0) + v_{\text{prop}}t$ observed in the 2D lake problem. The active rod hits the wall at time t_{wall} such that $\rho(t_{\text{wall}}) = R/2$, and, using the expression for $\rho(t)$ above, we get

$$t_{\text{wall}} = \frac{R}{\theta_0 v_f} \left(\exp \left(\frac{v_f}{2v_{\text{prop}}} \right) - 1 \right).$$

Thus, we conclude that as the active rod aligns more and more with the flow, its ability to move radially toward the wall diminishes because the radial component of its velocity becomes too small. In particular, the time it takes to reach the wall grows exponentially with the flow rate v_f .

We complete the analysis of the 3D river problem by showing that an accumulated active rod does converge for $t \rightarrow \infty$ to the wall location where the orientation of its cross-sectional projection (normalized) coincides with the outward normal. Note that in the case of zero rotational diffusion, the active rod swims along the wall for all times and can never escape the wall. The dynamics of the accumulated rod can be described by the following system whose derivation is relegated to Supplemental Material [46]:

$$\begin{aligned} \dot{\theta} &= -\frac{2v_f}{ab} J(\alpha) \sin^2(\theta) \cos(\psi), \\ \dot{\alpha} &= v_{\text{prop}}(J(\alpha))^{-1} \sin(\theta) \sin(\psi), \\ \dot{\psi} &= -abv_{\text{prop}}(J(\alpha))^{-3} \sin(\theta) \sin(\psi). \end{aligned} \quad (18)$$

The variable $\alpha(t)$ parameterizes the position of the accumulated active rod along the wall, with coordinates given by $(x, y) = (a \cos \alpha, b \sin \alpha)$. The variable $\psi(t)$ denotes the angle between the outward normal vector $\mathbf{n}$ of the wall and the (x, y) projection of the active rod's orientation vector $\mathbf{p}$, given by $(\mathbf{I} - \mathbf{e}_z \mathbf{e}_z^T) \mathbf{p}$. Here, $J(\alpha) = \sqrt{b^2 \cos^2(\alpha) + a^2 \sin^2(\alpha)}$ is a smooth function and $b \leq J(\alpha) \leq a$. Convergence to the wall location, where the outward normal vector is colinear with the (x, y) projection of the active rod orientation vector, is equivalent to the condition $\psi(t) \rightarrow 0$ as $t \rightarrow \infty$. This limit follows from the following observations.

First, since the rod remains accumulated at the wall, we have $-\pi/2 < \psi(t) < \pi/2$, which implies $\cos(\psi(t)) > 0$.

Furthermore, because $\sin(\theta(t)) > 0$, we obtain

$$\frac{d}{dt} [\cos(\psi)] = abv_{\text{prop}}(J(\alpha))^{-3} \sin(\theta) \sin^2(\psi) \geq 0.$$

It follows that $\cos(\psi) \geq \cos(\psi_0) > 0$, where ψ_0 denotes the initial value of ψ when the rod first accumulated at the wall.

Second, from the equation for θ in Eq. (18), we have the inequality

$$\dot{\theta} \geq -g \sin^2(\theta), \quad \text{where } g = \frac{2v_f}{b}.$$

Solving this differential inequality yields

$$\theta(t) \geq \cot^{-1}(gt + \cot(\theta_0)).$$

Using the inequality $\cot^{-1}(z) > \frac{1}{z+1}$ for $z > 0$, we further obtain $\theta(t) \geq (gt + \cot(\theta_0) + 1)^{-1}$.

Since $\theta(t) \rightarrow 0$ as $t \rightarrow \infty$, it follows that

$$\int_0^\infty \sin(\theta(t)) dt = \infty. \quad (19)$$

Third, the function $\psi(t)$ must retain a constant sign for all $t > 0$; it cannot switch between positive and negative values. Without loss of generality, assume $\psi(t) > 0$ for all $t > 0$. Then, from the equation for ψ in system (18), we have

$$\frac{\dot{\psi}}{\sin(\psi)} \leq -\frac{bv_{\text{prop}}}{a^2} \sin(\theta).$$

Integrating both sides gives

$$\frac{\tan(\frac{\psi(t)}{2})}{\tan(\frac{\psi_0}{2})} \leq \exp \left\{ -\frac{bv_{\text{prop}}}{a^2} \int_0^t \sin(\theta(\tau)) d\tau \right\}.$$

Taking the limit as $t \rightarrow \infty$ and using Eq. (19), we conclude that $\tan(\frac{\psi(t)}{2}) \rightarrow 0$ and thus $\psi(t) \rightarrow 0$.

Finally, based on the analysis above, we conclude that active rods in both the 2D lake and 3D river problems, in the case of $\hat{D}_{\text{rot}} = 0$ and $\mathcal{T} = 0$, eventually accumulate at the normal-to-wall position. Their steady-state distribution is given by $f(\alpha)$ as defined in Eq. (15), assuming the active rods are initially distributed uniformly at random. In the 3D river case, the presence of background flow tends to align the active rods with the axis of the microchannel, thereby reducing their radial velocity toward the wall, and the time required for wall accumulation can be significantly extended and scales exponentially with the flow rate.

Next, we consider various $\hat{D}_{\text{rot}} \geq 0$ and perform numerical simulations of the active rod under confinements. The Fig. 2 depicts the results of numerical simulations for $N = 500$ rods whose swimming is confined by the microchannel wall ∂M . As evident from this figure (see also SM video 1 [46]), most of the rods accumulate at the wall and swim upstream, which is the well-known feature of active swimming [27]. The background flow vanishes at the wall due to no slip boundary conditions, thus the speed of active rods swimming upstream at the wall is close to the propulsion speed v_{prop} . Active rods swimming downstream near the centerline where the $\mathbf{u}$ is maximum have speed $|\mathbf{u}| + v_{\text{prop}}$. As the result, right after simulation starts, two distinct profiles of active rods emerge. The first one is the downstream parabolic profile whose spreading speed depends on the flow rate, and

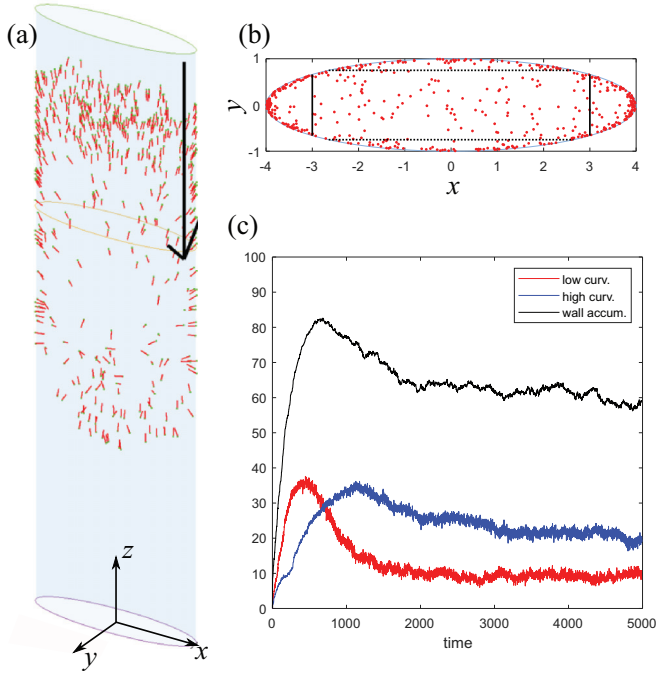


FIG. 2. Transport of active rods in an elliptic microchannel with $a = 4$ and $b = 1$. Active rods are initiated with $z = 0$, random coordinates x, y and orientation angles φ and θ . In subfigure (a), $N = 500$ active rods are depicted as red segments with the green edge on the active rod's front. The subfigure shows active rods' configurations after 1000 simulation time step. Black downward arrow shows the direction of the background flow $\mathbf{u}$. Purple (bottom), yellow (middle), and green (top) elliptical rings are at $z = -20$, $z = 0$, and $z = 10$, respectively. Subfigure (b) depicts projections of active rods' centers onto x, y plane as thick red dots. Black solid and broken lines are given by $x = \pm n_a$ and $y = \pm n_b$, respectively. Subfigure (c) depicts fraction (out of 100%) of accumulated rods (wall accum.), accumulated rods in M_a (high curv.), and accumulated rods in M_b (low curv.). An active rod is considered accumulated if its front touches the microchannel's wall.

this profile quickly dissolves as active rods turn toward the wall. The second one is the upstream flat profile with a constant speed independent from the flow rate. These profiles and how they depend on the flow rate can be observed in SM video 2 [46]. A typical individual trajectory of an active rod consists of alternating intervals of swimming upstream at the wall and downstream inside the channel. Note that an active rod can escape from the wall into the channel only by random reorientation accounted by the rotational diffusion term in Eq. (6b). At the same time, the background flow exerts the maximal torque at the wall where shear rate, $|\nabla \mathbf{u}|$, is the highest. This torque is the reason of the upstream swimming (the negative rheotaxis) at the wall but it cannot lead to the escape of the active rod from the wall since this torque vanishes as the active rod becomes tangential to the wall.

Active rods accumulate along lines where the wall curvature is highest, $(\pm a, 0, z)$. To measure the ratio between number of rods accumulated at the highest curvature locations $(\pm a, 0, z)$ and the lowest curvature locations $(0, \pm b, z)$, we count active rods inside domains $M_a = M \cap \{|x| > n_a\}$ and

$M_b = M \cap \{|y| > n_b\}$. Domains M_a and M_b can be understood as vicinities inside the microchannel of locations $(\pm a, 0, z)$ and $(0, \pm b, z)$, respectively. Numbers n_a and n_b are chosen in a such way that M_a and M_b have the same area when projected onto x, y -cross-section Ω . One can show that this definition of n_a and n_b implies $n_a/n_b = a/b$. Figure 2(c) shows the count of accumulated rods as a function of time. The fractions of accumulated rods and rods accumulated inside M_a and M_b were stabilized after approximately 1500 time steps indicating that the rod's distribution converged to a steady state. The fraction of rods accumulated at points of highest curvature, that is, inside M_a , is almost twice as large as the fraction of rods at points of lowest curvature, that is, inside M_b . It is worth noting that the wall area in M_b is larger than in M_a . Indeed, the length of elliptical curves for projections of M_a and M_b in Fig. 2(b) are approximately 2.52 and 5.32, respectively. Still, there are more accumulated rods at the wall in M_a than in M_b , as shown in the graph of Fig. 2(c). We also note that the accumulation fractions shown in Fig. 2(c) exhibit nonmonotonic behavior during the transient period (less than 1500 time steps). To explain this nonmonotonicity, recall that the velocity component in the cross-sectional (x, y) plane has magnitude $v_{\text{prop}} \sin(\theta)$. A larger value of this component leads to faster accumulation of active rods. Initially, the angle θ is uniformly distributed, resulting in relatively high cross-sectional velocities and rapid accumulation. As time progresses, and as confirmed by our analysis, the distribution of θ becomes concentrated around 0 and π , which reduces the cross-sectional velocity and leads to slower accumulation.

To illustrate how the distribution of accumulated active rods varies with dimension (2D versus 3D), rotational diffusion, and the presence of an extruding flow $\mathbf{u}$, we computed histograms of the locations of active rods at the wall; see Fig. 3. We parametrize the wall cross-section $\partial\Omega$ as $x = a \cos(\alpha)$, $y = b \sin(\alpha)$, where $\alpha \in [-\pi, \pi)$. Note that $\alpha = 0, \pm\pi$ and $\alpha = \pm\pi/2$ correspond to points of maximum and minimum curvature, respectively. For the i th active rod, if the rod is accumulated at the wall, then its front lies on the boundary and its location can be expressed as $(a \cos(\hat{\alpha}_i), b \sin(\hat{\alpha}_i))$ for a unique $\hat{\alpha}_i$. In the case of the 2D lake problem without rotational diffusion, the resulting histogram approximates the distribution $f(\alpha)$ from Eq. (15), as expected. As rotational diffusion increases, the distribution transitions toward a more uniform profile. This effect is even more pronounced in the 3D river problem, particularly when an extruding flow is present. In this case, the flow aligns active rods with streamlines, which hinders their lateral movement toward the wall. In all four cases, peaks consistently appear at $\alpha = 0$ and $\alpha = \pm\pi$, corresponding to regions of highest curvature.

B. Dependence of the active rod accumulation on the flow rate, the diffusion coefficient, and the aspect ratio of the microchannel cross-section

To quantify the active rod accumulation we calculate the time fraction spent swimming at the wall, that is, the average percentage of time that an active rod spends at the wall. Note that an equivalent definition of the time fraction is the time average of the wall accumulation depicted as a black graph in Fig. 2(c).

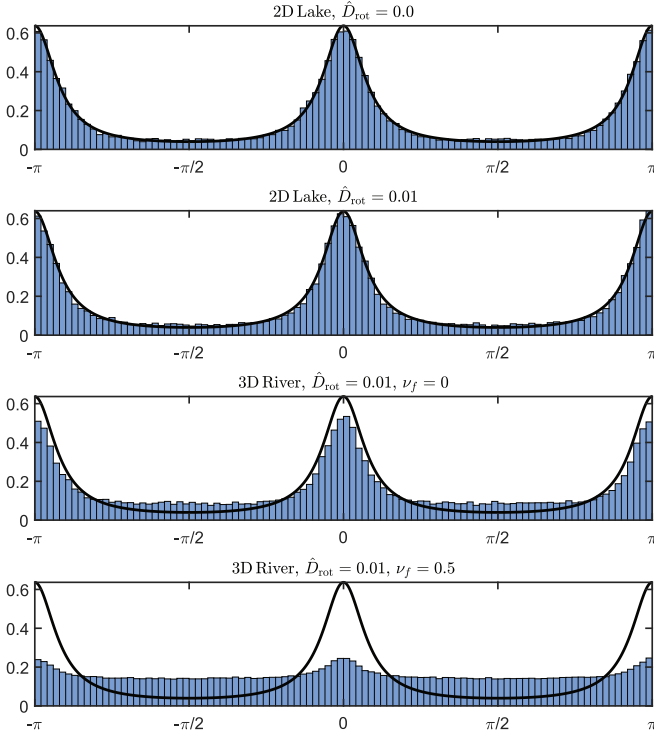


FIG. 3. Large-time distribution of accumulated active rods at the wall parameterized with the parameter α for both the 2D lake and the 3D river problems. The number of active rod simulations used to construct the histograms is $N = 50\,000$ for the 2D lake problem and $N = 20\,000$ for the 3D river problem. A smaller number of simulations is used for the 3D case to reduce computational cost. All four cases were simulated for 100 000 time steps. Only accumulated rods, defined as those in contact with the wall, are considered in the analysis. For the 2D lake case, histograms are based on the final positions of accumulated rods at the end of the simulations. In contrast, for the 3D river problem, wall-contact positions of active rods are recorded at time points $T_n = 1000 \times n$ for $n > 3$, after observing that the distribution of active rods has reached a fluctuating equilibrium state by $T_3 = 3000$ time steps. A longer sampling period is required in the 3D river case due to its slower accumulation rate (see also Fig. 4), compared to the 2D lake problem. Consequently, and because of the smaller total number of simulations (N), the effective sample size for the 3D river problem is significantly lower than that of the 2D lake case, particularly if sampling is limited to wall-contact positions at the end of the simulation. For an accumulated active rod, the parameter α is computed based on the location of its front touching the wall (x_f, y_f) : $\alpha = \text{atan2}(y_f/b, x_f/a)$. In all four subfigures, the number of bins is 100 and the black solid line corresponds to the distribution $f(\alpha)$ from Eq. (15). Horizontal axis is for parameter α , and histograms are normalized so the total area of bars is 1.

We first note that the concentration of active rods at the wall location with the highest curvature is observed without a background flow. However, in the absence of background flow, we no longer observe negative rheotaxis or the asymmetric spreading characterized by an upstream flat and downstream parabolic profile, as there is no upstream or downstream swimming without a background flow. As shown in Fig. 4 (left), the maximum accumulation occurs near the zero flow rate and decreases as the flow rate is increased.

This decrease is expected: as the flow rate increases, the ratio of self-propulsion to flow rate, $v_{\text{prop}}/|w(0, 0)|$, decreases. At high flow rates, active rods behave like passive rods, following streamlines and not accumulating. Therefore, the time fraction will decay to 0 as the flow rate goes to ∞ . Nevertheless, for small flow rates we also observe that the average accumulation time does not change significantly. The role of the background flow in active rod accumulation cannot be reduced to merely the decrease of the accumulation. We observe that the time fraction for accumulation in the low curvature domain M_b grows with the flow rate until the flow rate is approximately 0.5. Concentration at the high curvature locations drops down with the flow rate, as it is seen in the inset of Fig. 4 (left).

Active rod accumulation decreases as the rotational diffusion $\hat{D}_{\text{rot}}$ increases [see Fig. 4 (center)]. For zero rotational diffusion ($\hat{D}_{\text{rot}} = 0$), if an active rod collides with the wall, it remains there indefinitely because neither the background flow nor rod-wall interactions can reorient the rod toward the interior of the microchannel. In other words, since all active rods eventually collide with the wall, the time fraction, if computed over a time interval starting long after the initial time step, will be close to 100% for $\hat{D}_{\text{rot}} = 0$. The observed time fraction for $\hat{D}_{\text{rot}} = 0$ is approximately 83%, which is notably less than 100%. This discrepancy occurs because the time fraction is calculated over a period that includes the initial moment when active rods are randomly generated, mostly away from the wall, and thus require some finite time to collide with the wall. As $\hat{D}_{\text{rot}}$ is increased from 0, accumulation values drop down quickly. Namely, the time fraction halves for $\hat{D}_{\text{rot}} = 0.03$ compared to results for $\hat{D}_{\text{rot}} = 0$. Interestingly, despite the decrease in the total accumulation as we increase $\hat{D}_{\text{rot}}$, the ratio between accumulations at high and low curvature locations is nonmonotonic with a peak at $\hat{D}_{\text{rot}} \approx 0.1$, as visible in the inset of Fig. 4 (center).

Finally, we investigated how the total accumulation and the ratio between accumulations at high and low curvature locations depends on the eccentricity of the microchannel cross-section, $e = \sqrt{1 - b^2/a^2}$ [see Fig. 4 (right)]. For the sake of comparison, we keep ab constant so that the volume of the fluid passing through a microchannel cross-section per unit of time v_e is the same. Keeping ab constant also implies that we consider the same cross-sectional area. Introducing $s = ab$, we find expression of a and b in terms for s and e :

$$a = s^{1/2}(1 - e^2)^{-1/4} \quad b = s^{1/2}(1 - e^2)^{1/4}.$$

We fix the area parameter $s = 4$ and increase eccentricity e from 0 to 0.99. We see in Fig. 4 (right) that the time fraction of active rods accumulating at wall stays constant for a wide range of eccentricities, $0 \leq e \lesssim 0.95$. Time fractions for M_a and M_b are the same if $e = 0$, that is $a = b$, which is expected since $e = 0$ means that the cross-section is a circle and, thus, M_a and M_b have the same shape. As we increase eccentricity e we see the discrepancy between accumulations in M_a and M_b , but this discrepancy decreases as the total accumulation begins to decrease. This decrease is presumably due to the small shear rate values, $|\nabla w|$, near $x = \pm a$ when the eccentricity e is close to 1, resulting in weaker alignment with the flow at these locations [see, e.g., the equation for θ in Eq. (12)].

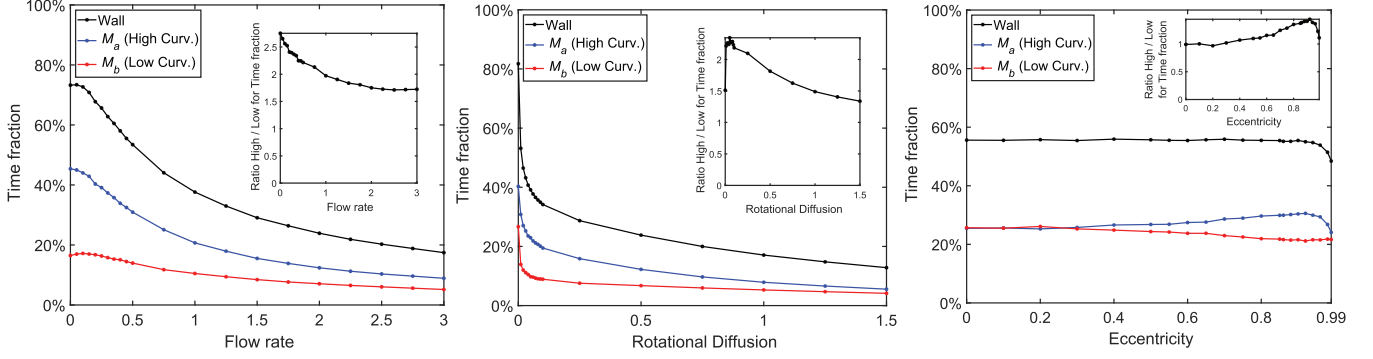


FIG. 4. Active rod accumulation dependence on flow rate, rotational diffusion coefficient, and microchannel eccentricity. Simulations are performed for $N = 20000$ rods. Time fraction in all three subfigures is the average number of time steps when a rod collides with the wall [when $q = 1$ in Eq. (13) or, equivalently, when the front of the rod ends up outside the microchannel and adjustments described below (13) are applied] divided by the total number of time steps. The average is taken over all N rods. The time fraction is expressed in percentages. Typical values of flow rate, diffusion coefficient, and eccentricity are 0.5, 0.01, $\sqrt{15}/4 \approx 0.97$, respectively. When varying one of these three parameters, the other two are held at their typical values. The subfigures also depict time fractions for collisions with the wall inside the domain M_a , containing the highest curvature locations (in blue), and M_b with the lowest curvature locations (in red). Insets show the ratio between time fractions for M_a and M_b . In the left subfigure, the flow rate is defined as $|w(0, 0)|$ where w is the solution of Eq. (10). The rotational diffusion in the center subfigure is the coefficient $\bar{D}_{\text{rot}}$ from Eq. (6b). When varying eccentricity (the right subfigure), we keep ab constant, specifically at $ab = 4$. We simulate more values of the flow rate and rotational diffusion coefficient at values close to 0, and eccentricity close to 1 (but excluding 1 since Ω has no interior in this case) to accurately capture the trend at these parameter limits.

C. The dynamics of the active rod exhibit a bifurcation with respect to the wall torque parameter $\mathcal{T}$, showing strong high-curvature accumulation in the subcritical case and reduced accumulation in the supercritical case

To study the boundary accumulation dynamics in the case $\mathcal{T} > 0$, that is, when the wall torque is taken into account [recall that the parameter $\mathcal{T}$ was introduced in Eq. (14)], we first consider the two-dimensional setting (the lake problem) with no rotational diffusion. The lake problem reveals a non-trivial effect of the wall torque on dynamics of active rods accumulated at a curved surface. First, we note that if the wall is planar, then introduction of the wall torque makes the orientation $\mathbf{p} = \mathbf{n}$ unstable, regardless of how small the parameter $\mathcal{T} > 0$ is. Surprisingly, the orientation $\mathbf{p} = \mathbf{n}$ can be asymptotically stable for $\mathcal{T} > 0$ when the wall has a nonzero curvature. Namely, there is a critical value of the wall torque parameter $\mathcal{T}_{\text{crit}} > 0$ at which a pitchfork bifurcation occurs causing active rods to become stuck at the wall with $\mathbf{p} = \mathbf{n}$ in the subcritical case $\mathcal{T} < \mathcal{T}_{\text{crit}}$ (see also and SM video 5 [46]). For example, consider an active rod swimming in the circular lake Ω of radius R . Suppose that the active rod has collided with the wall so that its dynamics occurs along the wall. As in the system (18), let $\psi(t)$ denote the angle between the orientation vector $\mathbf{p}$ of the active rod and the outward normal vector $\mathbf{n}$ at the wall location where the active rod touches the wall at time t . If $\psi = 0$, then the rod is perpendicular to the wall and neither swims nor reorients. Angles $\psi = \pm\pi/2$ correspond to swimming tangent to the wall. We show in Supplemental Material [46] that $\psi(t)$ satisfies the following differential equation:

$$\dot{\psi} = \frac{6v_{\text{prop}}}{\ell} \sin(\psi) \left(\mathcal{T} \cos(\psi) - \frac{\ell}{6R} \right). \quad (20)$$

If we fix v_{prop} , ℓ , and R , then this differential equation exhibits a pitchfork bifurcation at $\mathcal{T}_{\text{crit}} = \ell/(6R)$. If $0 \leq \mathcal{T} \leq \mathcal{T}_{\text{crit}}$,

then the active rod eventually accumulates at the wall with $\psi = 0$ and swimming ceases. If $\mathcal{T} > \mathcal{T}_{\text{crit}}$, then $\psi = 0$ is unstable and $\psi(t)$ converges to $\pm \arccos(\mathcal{T}_{\text{crit}}/\mathcal{T})$ meaning that the active rod will swim along the wall, either clockwise or counterclockwise, at an angle relative to the wall (see Figs. 5(a) and 5(b) and SM video 6 [46]). If we formally pass to the planar limit $R \rightarrow \infty$, then $\mathcal{T}_{\text{crit}}$ vanishes so $\psi = 0$ is unstable for all $\mathcal{T} > 0$ and the two stable angles are $\pm \arccos(0) = \pm\pi/2$, that is, swimming tangent to the wall. Finally, we note that this bifurcation phenomenon can lead to formation of trapping regions around high curvature points in the elliptical domain Ω . Specifically, because the value of R is inversely proportional to the curvature, the critical value $\mathcal{T}_{\text{crit}}$ increases with the curvature. If $\mathcal{T}$ is fixed, then in an elliptical wall where curvature varies, it may happen that regions with higher curvature have $\mathcal{T} < \mathcal{T}_{\text{crit}}$ so $\psi = 0$ becomes stable, and active rods stop swimming (forming the trapping region), whereas locations with lower curvature have $\mathcal{T} > \mathcal{T}_{\text{crit}}$ allowing active rods to maintain a certain speed along the wall and eventually clear the low-curvature regions. An example of such a case is presented in Fig. 5(d) and SM video 5 [46].

Finally, we performed numerical simulations in the three-dimensional settings for the case $\mathcal{T} > 0$. We varied $0 \leq \mathcal{T} \leq 1$, with other parameter values kept the same as in Fig. 4. As shown in Fig. 6, increasing $\mathcal{T}$ results in a decrease of the accumulation of active rods. The wall torque also accelerates the transport of accumulated rods along the wall surface, see also SM video 3 [46]. For nonsmall values of $\mathcal{T}$, the wall torque term (14) reorients an accumulated active rod to a direction tangent to the wall surface. When an active rod is oriented tangentially to the wall, it swims faster along the wall, as this speed is proportional to the projection of the direction vector $\mathbf{p}$ onto the tangent plane. In contrast, an active rod that is almost perpendicular to the wall swims more slowly along the wall. Additionally, tangential swimming increases

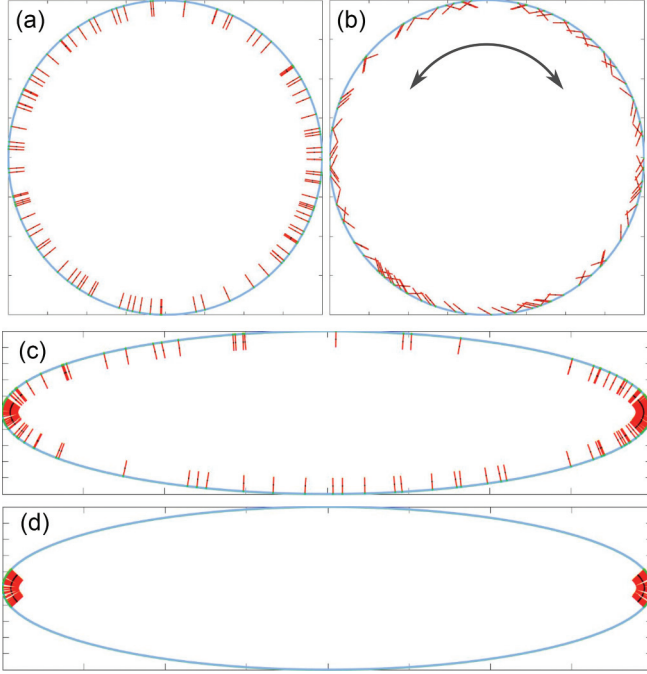


FIG. 5. Illustration of the bifurcation phenomenon with respect to the wall torque parameter $\mathcal{T}$ in the two-dimensional settings. All four subfigures depict large time configurations: in panels (a), (c), and (d) active rods arrive to their equilibrium position $\mathbf{p} = \mathbf{n}$, whereas in panel (b) active rods constantly moving both clockwise and counterclockwise, as the arrow shows. In subfigures (a) and (b), we compare the subcritical case, active rods remain stationary and oriented perpendicular to the wall, to the supercritical case where active rods are moving steadily with a tilting angle. Subfigures (c) and (d) illustrate high curvature accumulation of active rods for $\mathcal{T} = 0$ and $\mathcal{T} = 0.1$. Subfigures (a, b) are taken from SM video 6 [46], whereas panels (c) and (d) are from SM videos 4 and 5 [46], respectively.

the likelihood of the active rod escaping from the wall due to random reorientation and thus reduces the wall accumulation. Hence, the wall torque for nonsmall values of $\mathcal{T}$ reduces the accumulation of the active rod wall.

IV. DISCUSSION

Our results characterize both the wall and high curvature accumulation of active swimmers in a three-dimensional microchannel with an extrusion flow. In particular, straight lines on the cylindrical wall, parallel to the microchannel's major axis and corresponding to high-curvature wall locations, have a trapping effect on the dynamics of individual active rods, which can be utilized to control and guide microswimmers. We hypothesize that corners act as stronger attractors for active rod concentration compared to locations with finite curvature. Specifically, our model captures the four-lane structure of active swimmer dynamics in microchannels with a rectangular cross-section, see SM video 7 [46]. This four-lane structure indicates that active swimmers tend to move along the four corners of the microchannel, a phenomenon observed in experiments [15,35,36]. The accu-

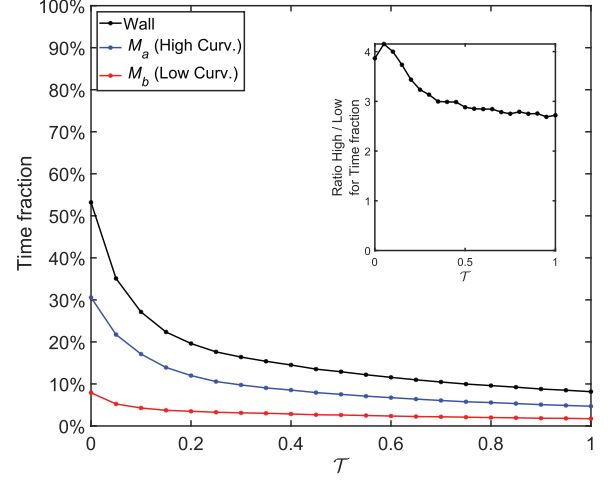


FIG. 6. Dependence of active rod accumulation on the wall torque $\mathcal{T}$. Settings are the same as in plots from Fig. 4.

mulation of active rods may also depend on the angle of the corner, which can be tested using the model presented in this work.

However, the presence of an extruding flow and the resulting rheotaxis, which aligns the swimmer with the streamlines parallel to the walls, significantly prolong the initial descent of an active rod toward the wall. While the results presented in this work focus on the dynamics of individual active rod swimming, the inclusion of interactions between active rods, such as steric and hydrodynamic interactions, is expected to give rise to collective phenomena modulated by confinement [48–50]. The form of hydrodynamic interactions depends on the type of microswimmer represented by the active rod, whether it is a pusher or a puller [25,33]. In the context of the dilute suspensions considered in this work, the accumulation of active rods leads to the emergence of two distinct phases within the population: a high-density liquid phase near the wall and a low-density gas phase in the bulk. This behavior resembles the well-known phenomenon of motility-induced phase separation observed in active Brownian particles [51,52], which arises from collective effects and does not require confinement. However, the phase separation can be significantly altered by the introduction of an extrusion flow in the presence of confinement, which is relevant for practical applications.

One immediate consequence we can anticipate is that a population of interacting active rods with wall torque $\mathcal{T} > 0$ may exhibit collective motion, swimming coherently in either the clockwise or counterclockwise direction around the major axis of the microchannel. In contrast, a single, noninteracting rod has equal probabilities of choosing either direction. Furthermore, it is important to understand how rod-rod interactions influence the number of rods that escape from wall entrapment. Future work will extend the current framework to incorporate inter-particle interactions and investigate the emergence of collective behaviors in various confinement geometries under extrusion flow.

To draw strong conclusions about active rod accumulation for different geometries, a kinetic approach is required. This involves solving a partial differential equation where

the unknown is the distribution function of the active rods' location and orientation. Unlike Monte Carlo simulations, this approach is deterministic. Such an approach, which also explicitly distinguishes between the distributions of active rods at the wall and away from it, has been developed in Refs. [53,54] for the two-dimensional case (where the wall is a curve). Implementing this approach for a three-dimensional cylindrical microchannel presents challenges due to the need to handle differential operators over surfaces (the unit sphere for orientation $\mathbf{p}$ and the wall surface) and singular terms that

describe active rods detaching from the wall. Developing a robust numerical scheme for this equation will enable testing and comparison of various microchannel geometries and help elucidate the effects of curvature and corners on different types of microswimmers.

ACKNOWLEDGMENT

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