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Effective Diffusion Coefficient and Average Drift Velocity for a Bioinspired Drift Ratchet

J. Herringer[1], G. Dorrington[1] and G. Rosengarten[1]

[1]School of Aerospace, Mechanical and Manufacturing Engineering
RMIT University, Melbourne, Victoria 3053, Australia

Abstract

Diatoms are microscopic, phototrophic, unicellular algae encased in a porous, rigid, siliceous, cell wall known as the frustule. They inhabit the euphotic zones in bodies of seawater and freshwater. The nutrient and trace element sorting characteristics of the diatoms frustule is not yet fully understood. It has been proposed that the girdle band pores of the marine diatom species (*Coscinodiscus sp.*) uses the drift ratchet mechanism to sort and separate nutrients and trace elements from harmful particles (i.e. viruses), based on the particle size. From initial numerical simulation results the girdle band pores do exhibit drift ratchet behaviour for a range of fluid flows. The theory requires further comprehensive analysis of the girdle band pores be undertaken, as the hydrodynamic and thermal environment in which the diatom exist is not understood as of yet.

Introduction

Diatoms

The diatom species, *Coscinodiscus sp.*, is a single-celled, photosynthesising, microscopic algae [1]. They inhabit the region of oceans in the depth range at which sunlight penetrates to facilitate photosynthesising [1]. These phytoplankton surround their cell membrane with a rigid, transparent, porous, amorphous silica based shell — known as a frustule [17], similar to that shown in figure 1.

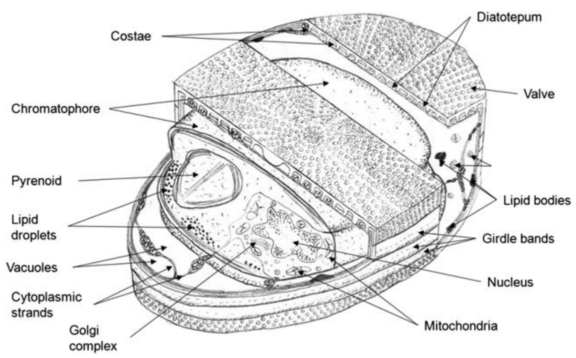

Figure 1. Schematic of a generic centric diatom [20]. The general diameter of the frustule of *Coscinodiscus sp.* is in the range of approximately 80-150 μm [17, 10].

It has been proposed that diatoms utilise their porous silica shell (among other proposed functions [15]) to sort and filter nutrients and trace elements vital for their survival and growth (i.e. NH_4^+, HCO_3^-, NO_3^- etc.), from harmful entities (i.e. bacteria and viruses) [10, 12].

This paper investigates whether *Coscinodiscus sp.* uses the drift ratchet phenomenon to prevent harmful particles (i.e. a virus) diffusing through its girdle band pores.

Drift Ratchet

A drift ratchet is a type of Brownian ratchet [7, 11]. To explain how a drift ratchet works, take a straight axisymmetric / asymmetric micro–pore. The asymmetry of the pore is characterised with respect to the change in the diameter of the pore along the pore axis (figure 2).

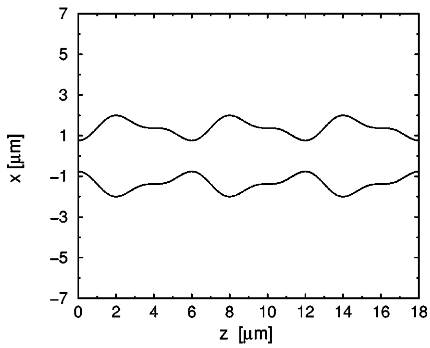

Figure 2. Schematic of the profile (along the pore axis – z-axis) of a drift ratchet studied by Kettner et al. [7].

If we then fill the pore with a fluid / micro–particle mixture (i.e. water as the continuum and micro–spheres as the solid phase) and introduce a temporally symmetric fluid oscillation inside the pore (i.e. zero average fluid displacement — so the fluid oscillates around a single position), then this scenario will give rise to net transport of particles in a single direction along the pore axis. The magnitude and direction of particle drift is dependent on the; shape of the pore, Brownian motion of the particles (i.e. particle size) and frequency and amplitude of the fluid oscillation [7, 11].
A drift ratchet operates at the microscopic scale where Brownian motion becomes a governing transport mechanism and the fluid flow is characterised by a low Reynolds number ($Re << 1$) which is dominated by viscous forces (i.e. inertial effects are negligible).

Losic et al. [9] identified geometric similarities between a drift ratchet pore investigated by [7, 11] and the pores of the girdle bands of the diatom *Coscinodiscus sp.* (figure 3 – Bottom).

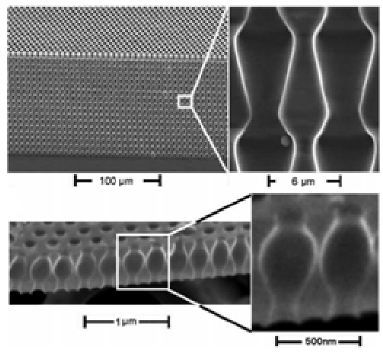

Figure 3. (Top) SEM of a massively parallel silica membrane with asymmetric pores [11]. (Bottom) SEM of girdle band pores of diatom *Coscinodiscus sp.* [9].

These girdle band pores (figure 3) are located in the mid-section of the frustule (figure 1). Although there may exist similarities between these pores there also exist differences driving this investigation. The diatom girdle band pores are smaller than the drift ratchet pores studied by [7, 11] (figure 2, figure 6 and table 1), the girdle band pores only have a maximum number of two repeating units in series compared to the 17-33 in series for the massively parallel drift ratchet membrane (figure 3 – Top), the girdle band pores also experience a different fluid oscillation condition based on what is experienced in their surrounding environment in the upper ocean.

Geometric feature	Drift ratchet	Girdle band
Max. diameter	$\approx 4\ \mu m$	$\approx 0.25\ \mu m$
Min. diameter	$\approx 1.5\ \mu m$	$\approx 0.1\ \mu m$
Length of a repeating unit	$6\ \mu m$	$0.5\ \mu m$
No. of repeating units in series	17-33	1-2

Table 1. Comparison of the pore profile geometry between the drift ratchet studied by [7, 11] and a girdle band pore. The profiles of each are shown in figure 2 and figure 6, respectively.

Rationale

It is estimated that diatoms generate 20% of the atmospheric oxygen and a majority of the biomass at the base of the food chain in the oceans around the world [14, 4, 6]. Diatoms act as a carbon sink (using carbon dioxide in photosynthesis) and are responsible for approximately 40% of the net primary carbon production in the ocean [5, 3]. It is therefore becoming critical to understand how these phytoplankton survive in such a competitive ecosystem because of the important role they play in such a system.
There also exists possible direct and indirect applications for diatom valves to improve the performance and efficiency of man-made filters and improve particle sorting characteristics of microfluidic devices [14].

The numerical simulation proposed in this paper is based on that developed by Kettner et al. [7] and will be verified by comparing results to that obtained by the same authors [7]. Two simulation cases (table 2) will be used to verify the algorithm, this will be covered in the section "Verification of Drift Ratchet Simulation". The verified simulation will then be used to analyse the case of a diatoms' girdle band pore geometry under the section "Girdle Band Pore Drift Ratchet Simulation".

Verifying Drift Ratchet Simulation

The governing equation (equation 1) used to model the drift ratchet simulation presented in this paper is similar to the Langevin equation used by Kettner et al. [7]

$$\vec{x}_{particle}(t) = \vec{x}_{fluid}(\vec{x}(t), t) + \sqrt{2D_{th}\Delta t}\vec{\gamma} \qquad (1)$$

where $\vec{x}_{particle}(t)$ and $\vec{x}_{fluid}(\vec{x}(t), t)$ is the particle and the fluid parcel displacement respectively over a single time step, $D_{th} = k_B T / 6\pi r \mu$ is the thermal diffusion coefficient and $\vec{\gamma}$ is a vector of random numbers from a standard normal distribution.

The drift ratchet simulation uses a progressive code to calculate the displacement of the particle, as a result of its Brownian motion and the fluid velocity, at each time step (Δt). To ensure accurate representation of both these displacements a small time step needs to be taken. A time step of $\Delta t = 10^{-6}$ s was used. Each simulation is run for a total simulation time (t_{run}) with a single particle in an infinite pore. Particle–particle interactions and the effect of finite pore length and basins at either end are not taken into account.

The fluid velocity was estimated by using an approximate solution to the stream function for an axisymmetric pore as shown in equation 2 (sourced from [7])

$$\Psi(r,z) = c - \frac{1}{2}\left(\frac{r}{r_p(z)}\right)^2 + \frac{1}{4}\left(\frac{r}{r_p(z)}\right)^4 \qquad (2)$$

where c is a constant, r is the radius inside the pore and $r_p(z)$ is the radius of the pore wall, which is a function of the position along the pore axis (z). This expression is only valid for small perturbations of the pore wall along the pore axis. Kettner et al. [7] used this approximation to then numerically derive a more representative stream function for their simulation. Only the above approximate solution was used in the current analysis.

The unperturbed velocity field was not integrated over the volume of a spherical particle, as was completed by Kettner et al. [7]. Instead only the unperturbed fluid velocity at the centre-point of the particle was used in equation 1 at a specific time step and position in the pore. Two-way coupling between the fluid and the solid particle phase has not been included either in the current study or by Kettner et al. [7].

The model used to represent the elastic particle–wall interaction is illustrated in figure 4.

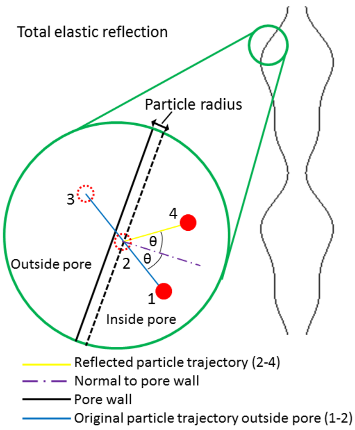

Figure 4. Schematic of how the particle–wall interactions are represented in the model currently being developed. The length of points 2-3 and 2-4 are equal.

The parameters used in the two cases to verify the new drift ratchet simulation are defined in table 2.

Parameters	Case 1	Case 2
Fluid amplitude (A)	$6\ \mu m$	$12\ \mu m$
Flow rate (Q_z)	$2426.5\ \mu m^3.s^{-1}$	$4853\ \mu m^3.s^{-1}$
Fluid frequency (f)	40 Hz	
Viscosity (μ)	$0.5\mu_{water}$	
μ_{water}	1.025×10^{-3} N.s.m^{-2}	
Temperature (T)	293 K	
Particle radius (r)	$0.35\ \mu m$	
Boltzmann constant (k_B)	1.38×10^{-23} m^2.kg.s^{-2}.K^{-1}	
Reynolds number ($Re_{\text{pore dia.}}$)	$0.004 - 0.008$	

Table 2. Parameters used in drift ratchet simulations by [7].

The fluid amplitude is the distance a fluid parcel travels along the centreline of the pore in half a period of oscillation. This set distance dictates the maximum volumetric flow rate required to satisfy this condition. The flow rate of the fluid oscillates sinusoidally.

To verify the new drift ratchet model against that of Kettner et al. [7] the average particle drift velocity (v_e) and the ratio of effective diffusion coefficient to thermal diffusion coefficient (D_e/D_{th}) were compared, defined by equation 3 and equation 4, respectively.

$$v_e = \frac{\langle z(t_{run}) \rangle}{t_{run}} \tag{3}$$

$$\frac{D_e}{D_{th}} = \frac{[\langle z^2(t_{run}) \rangle - \langle z(t_{run}) \rangle^2]}{2t_{run}} \times \frac{1}{D_{th}} \tag{4}$$

Where, $z(t_{run})$ is the displacement along the axis of the pore over a time period t_{run} [7]. $\langle \cdots \rangle$ is the average for many particle realisations.

Verified Results

The results (figure 5 and table 3) from the numerical model match well with the results published by Kettner et al. [7].

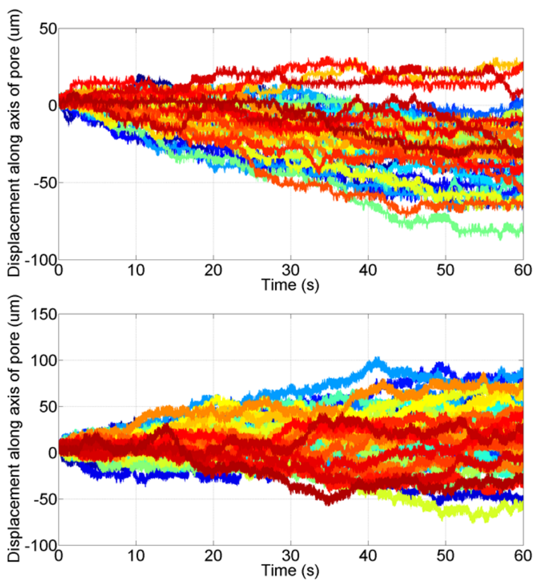

Figure 5. Displacement of a single particle along the axis of the drift ratchet pore illustrated in figure 2, using the model developed in this paper, for 50 separate particles. (Top) Case 1 and (Bottom) Case 2. The conditions of the simulation are as shown in table 2. The direction of displacement coincides with the orientation of the pore profile in figure 2. Initial position of all particles is at the origin.

	Case 1		Case 2	
	[7]	Current model	[7]	Current model
v_e (μm.s^{-1})	-0.45	-0.25	0.42	0.21
D_e/D_{th}	2.45	2.66	-	4.07

Table 3. Comparison of results between current drift ratchet model and that developed by Kettner et al. [7] for the 50 particles displayed in figure 5.

Girdle Band Pore Drift Ratchet Simulation

Now analysing the possible transport characteristics of a virus in a girdle band pore using the drift ratchet model will give us an idea if this drift ratchet mechanism can explain how harmful entities are prevented from penetrating the silica frustule.
The typical size of viruses which infect diatoms is of the order of 25-220 nm [13]. Assuming an approximate concentration of the above sized viruses in the upper ocean of 7×10^{11} m^{-3} [2] and using advection-diffusion encounter rates we can approximate the number of viruses meeting a single girdle band pore as 7 viruses every 5 minutes. Therefore the assumption of a dilute particle concentration inside the pore (negligible particle – particle interactions) is valid between viruses and diatoms in the ocean.

The diatom girdle band pores of *Coscinodiscus sp.* (figure 3 – Bottom) are defined schematically in figure 6.

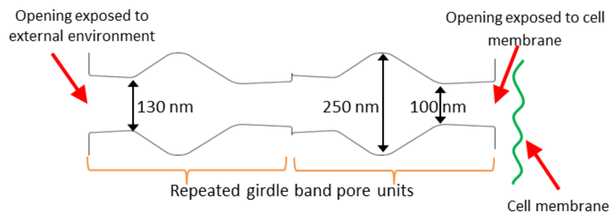

Figure 6. Schematic of the profile (along the pore axis) of the girdle band pores of the diatom *Coscinodiscus sp.*

A control simulation using a straight-walled pore (Case 4) is compared with the girdle band simulation (Case 3). The parameters for these cases are the same as that in Case 1 and Case 2 (table 2) except for the parameters included in the below table.

Parameters	Case 3	Case 4
Radius of pore wall	$r(z)$ (figure 6)	0.077 μm
Fluid amplitude (A)	6×10^{-3} μm	3×10^{-3} μm
Flow rate (Q_z)	1.35×10^{-4} μm^3.s^{-1}	
Fluid frequency (f)	1 Hz	
Water viscosity (μ)	9.59×10^{-4} N.s.m^{-2}	
Particle radius (r)	0.025 μm	
Pressure (ΔP)	1.21×10^{-2} Pa	
Reynolds number ($Re_{\text{pore dia.}}$)	$1\times10^{-9} - 1.7\times10^{-9}$	

Table 4. Parameters used in the girdle band simulations (Case 3) and the straight-walled model (Case 4).

Coscinodiscus sp., with a diameter of 140 μm, can sink through the water column at speeds of 81–347.5 μm.s^{-1} ($Re = 0.01 - 0.05$) [18]. These sinking speeds can induce a rotation of a non-spherical diatom with a period of 7.2–1.68 s. If we then explore the period range 10–1 s then we will gain a better understanding if these pores act like a drift ratchet [16]. The flow rate is approximated by using Poiseuille's Law, approximating a pressure drop across the ends of a straight-walled pore (the length of two repeating girdle band units) with a pore radius equal to the average radius from the girdle band profile. The pressure distribution around a sinking sphere experiencing Stokes flow is used to determine the pressure drop [19].

The results shown in figure 7 (Top) does not show preferential motion of a spherical particle (50 nm in diameter) and therefore does not support the hypothesis that the girdle band pores employ the drift ratchet mechanism.

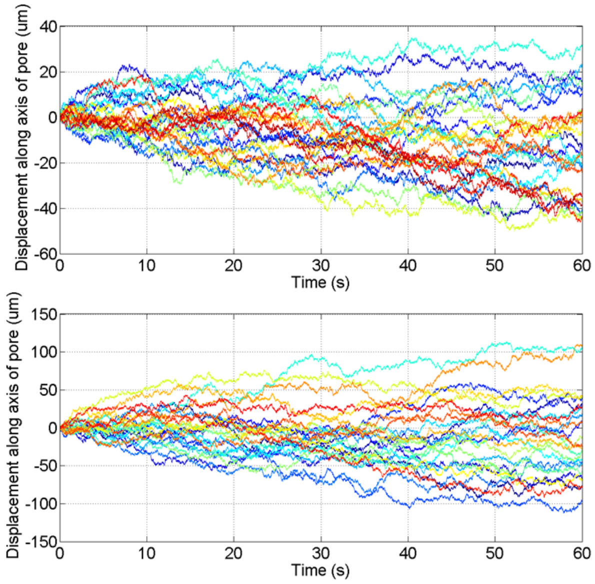

Figure 7. Displacement of a single particle along the axis of the girdle band pore illustrated in figure 6, using the model developed in this paper, for 25 separate occasions. (Top) Case 3 and (Bottom) Case 4. The conditions of the simulation are as shown in table 4. Negative displacement represents a displacement to the left in figure 6. Initial position of all particles is at the origin.

	Case 3	Case 4
v_e (μm.s^{-1})	-0.1	-0.11
D_e/D_{th}	0.23	1.35

Table 5. Comparison of results between girdle band pore profile (Case 3) and a straight-walled pore (Case 4).

When compared to the straight-walled pore, the girdle band pore hinders diffusion and does not provide biased drift of a particle in one direction (table 5).

For all the cases investigated the pore geometry and the Reynolds numbers are such that the flow inside the pore is attached and no recirculation regions form [8].

Conclusions

The hypothesis that this species of diatom uses the drift ratchet mechanism to sort particles based on their size cannot be discounted yet. Work is in progress to complete a parametric study.

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