Microfluidic simulation of a colonial diatom chain reveals oscillatory movement

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Diatoms are single-celled organisms with rigid parts in relative motion at the micro- and nanometer length scales. Some diatom species form colonies comprising many cells. In this manuscript, the results of a two-dimensional finite element computer model are presented. This model was established to discover if diatom colonies start to exhibit some kind of «pumping» behaviour when subjected to water flow. To analyze this computationally, a model diatom colony with continuously repeated units of ten cells is investigated in a fluid dynamic simulation. In this first simple model, undisturbed fluid flow is allowed for between the single cells. The cells do not move actively, and are solely moved by the water. The initial fluid velocity is assumed between 0.01 m s⁻¹ and 1 m s⁻¹. A computational result that does not change anymore with time is called a steady state solution. Such a steady state solution is reached in all calculations performed. The steady state for a chain where initially all diatoms are spaced equally (equidistant spacing) has forces that encourage the formation of cell pairs with less distance between one another. These forces result from the flow of the surrounding fluid. The steady state for a chain with initially paired cells shows the opposite effect: the pairs tend to un-pair and head for the equidistant state again. The mutual change in forces between these two states, i.e., paired and unpaired formations, suggests that these two steady states lead into each other: The computer simulations suggest that a diatom colony subjected to water flow exhibits some kind of oscillatory movement. Such movement might facilitate nutrient uptake of the diatom colony.

Keywords: Diatom chain, fluid dynamics, hydroelastics, nutrient uptake, computer simulation

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Introduction

Diatoms are single-celled organisms with rigid parts in relative motion at the micro- and nanometer length scales. The diatom frustule is a very rigid structure. This has been revealed by force measurements (HAMM et al. 2003, HAMM 2005, LOSIC et al. 2007). Adhesives produced by diatoms are modular, self-healing and extraordinarily tough (GEBES- HUBER et al. 2002, 2003; HIGGINS et al. 2002, 2003a, 2003b; DUGDALE et al. 2005). Such properties are the reason for increasing interest in diatoms for nano- and microtechnological applications (GEBESHUBER et al. 2005, in press; GORDON et al. 2005, 2009; CRAWFORD and GEBESHUBER 2006; GEBESHUBER and CRAWFORD 2006; GEBESHUBER 2007, GORDON et al. 2009). Some diatom species form colonies comprising many cells in the form of long chains (ROUND et al. 1990). *Rutilaria philipinarum* is an example of such a species (ROSS 1995). *R. philipinarum* is a fossil colonial diatom thought to have lived in inshore marine waters. In this species, the single diatoms connect by linking spines and by a complex siliceous structure termed the periplekton (Fig. 1). These linking structures on the one hand keep the cells together, but on the other hand also keep a distance between the cells. The shape of the spines allows expansion of the chain to a certain maximum distance and compression to a minimum distance, in which case there is still some fluid between the cells. The links allow movement of single cells in the chain against or from each other in a rather one-dimensional way (GEBESHUBER and CRAWFORD 2006). Such elaborated linking mechanisms inspired the question what would happen to such a diatom colony if it were subjected to water flow.

A diatom chain subjected to fluid flow orthogonal to its long axis is soon moved with the flow as a whole. However, in situations where the direction or velocity of flow changes, the inertia of the whole diatom chain prevents immediate acceleration according to new flow conditions. During the situation of acceleration, water flows through the gaps between the single cells creating relative motion between water and the chain.

To analyze the problem, the method of computational fluid dynamics (CFD) is used. CFD is one of the branches of that uses and algorithms to solve and analyze problems that involve fluid flows. The governing equations that need to be solved consider the conservation of mass, momentum, pressure and turbulence (LANDAU and LIFSHITZ 1987). Indeed, these equations are so closely coupled and difficult to solve that it was not until the advent of modern digital computers in the 1960s and 1970s that they could be resolved for real flow problems within reasonable timescales. Nowadays, CFD has become an indispensable part of the aerodynamic and hydrodynamic design process for planes, trains, automobiles, rockets, ships, submarines; and indeed any moving craft or manufacturing process that mankind has devised. A basic introduction to fluid mechanics for the interested reader is given by CHORIN and MARSDEN (1990). Numerical methods used to solve the governing equations in fluid mechanics can be found in LEVEQUE (2005).

The computer simulations presented here could inspire biologists working on diatoms to perform experiments validating the results, and thereby initiate interdisciplinary research involving groups from technical and biological backgrounds (GEBESHUBER and DRACK 2008).
Materials and methods

To prove the principle, a simple two-dimensional finite element model of a diatom chain has been created. This model chain does not contain linking spines or periplekton or surface textures of the diatoms, but solely concentrates on primary aspects concerning the boundary conditions of multiple gaps (Fig. 2). In the model, the diatom cell size is assumed to be 140 µm x 34 µm, and the distance between the cells can achieve a value from 10 µm to 20 µm. The colony is assumed to be comprised of single units of 10 cells each that are re-

Fig. 1. Schematic drawing of a chain of *R. philipinarum*, illustrating three single diatoms with the linking structures and the periplekton with its screw-like structure. The long spines arranged in a ring ensure a certain minimum distance between the single cells while connecting them to each other.

Fig. 2. The white boxes counted from A1 to A10 symbolize the model diatoms. The model diatoms have one degree of freedom of movement, namely in the ± y direction, indicated by the arrows in cells A5 and A6. The x- and y-axes of the coordinate system used are given on the right. The size of each model diatom cell is 140 µm x 34 µm, the distance between them is 15 µm. In the gaps between the boxes water flows in the direction marked with the bold arrows. The brighter area in the middle of the figure represents the «unit cell» of the endlessly repeated sequence, repeated units being indicated by the darker areas to the left and the right.
peated endlessly. This simplifies calculations, but does not provide any information about possible influences of the ends of the chain. The chain of model-diatoms is surrounded by water.

In all calculations, stationary solutions are sought. If the length of a model-diatom is chosen as a characteristic length scale, the Reynolds number ($Re$) turns out to be very low.

$$Re = \frac{\rho v L}{\eta}$$

Here $\rho$ describes the density ($1000 \text{ kg m}^{-3}$), $v$ the velocity (varied between 0.01 m s$^{-1}$ and 1 m s$^{-1}$), $\eta$ the dynamic viscosity ($1.003 \times 10^{-3} \text{ Pa s}$) of the surrounding water and $L$ is the assumed characteristic length ($140 \times 10^{-6} \text{ m}$). Therefore the maximum Reynolds number turns out to be $\sim 140$. This allows us to assume that the problem is laminar.

In this simple isothermal model (i.e. constant temperature), undisturbed fluid flow is allowed for between the single cells. The simulated fluid is water with a temperature of 293.15 K. The cells do not move actively, and are solely moved by the water. To simulate the fluid flow, boundary conditions are necessary. The inlet velocity of the fluid is varied between 0.01 m s$^{-1}$ and 1 m s$^{-1}$ in steps of an order of magnitude. As an outlet condition, an averaged static pressure of one bar is assumed. Assuming the diatom colony to comprise much more than ten cells justifies the other two boundary conditions as to be symmetry. In this way, the four boundary conditions needed for the two dimensional model are defined, and the problem is ready to be solved.

For solving the problem, the software package ANSYS CFX 11.0 is used. Similar to further commercial software packages ANSYS uses the finite-volume method, which is a standard technique where the equations are solved on discrete control volumes. The models consist of up to 308283 volumes. This mesh of elements is created in ANSYS ICEM CFD 11.0.

**Results**

In the simulations, steady state solutions (i.e. a computational result that does not change anymore with time) are calculated for two different arrangements of the model diatom chain (Fig. 2). There are two different possible directions of the fluid to flow: along the long axis of the chain in the $y$-direction or across the chain through the gaps in the $x$-direction. All other possible fluid flows are simple superpositions of these two cases. The first case, when the fluid flows along the chain, only reveals a simple elongation of the chain. This is the reason why this case has not been investigated any further.

On the other hand, fluid flow orthogonal to the long axis of the chain is worth examining in more detail: The first pre-set configuration investigated has equidistant model diatom cells (i.e. all model diatom cells have the same distance to their neighbouring cells, Fig. 3). This represents a balanced position of the diatoms in the chain. The second pre-set configuration investigated has alternating distances of the model diatom cells ($d_{\text{min}}$ between A1 and A2, $d_{\text{max}}$ between A2 and A3, $d_{\text{min}}$ between A3 and A4, $d_{\text{max}}$ between A4 and A5, and so on, with $d_{\text{min}}$ being 10 µm and being $d_{\text{max}}$ 20 µm). This arrangement is one single example for an imbalanced condition of the chain and is shown in figure 4. The resulting acting forces grow proportionally with the velocity but do not change in direction with the
different velocities investigated (0.01 m s\(^{-1}\)–1 m s\(^{-1}\)). Therefore, the influence of different incoming flow velocities turns out to be not significant for the specific behaviour investigated. Even though the acting forces in the flow direction (x-direction, Fig. 2, Tab. 1) are about a hundred times larger than the forces orthogonal to the flow direction (y-direction, Fig. 2, Tab. 1) for the equidistant state, it is mainly results for the forces orthogonal to the flow direction that are presented. The reason for this is that the solution for the forces in the x-direction is trivial: the whole chain of model diatoms accelerates in the direction of the flow.

Forces on the cells strongly correlate with the static pressure of the surrounding fluid, which again corresponds to the velocity of the fluid in the gaps due to Bernoulli’s principle. In fluid dynamics, Bernoulli’s principle states that for an in-viscous flow, an increase in the speed of the fluid occurs simultaneously with a decrease in pressure (e.g. LAMB 1994). Bernoulli’s principle is named after its developer Daniel Bernoulli (1700–1782).

**Equidistant model diatoms:** Figure 3 shows the result for an inlet flow-velocity of 0.1 m s\(^{-1}\) in the positive x-direction. The white boxes represent the model diatoms. The fluid velocity is coloured from blue (slow) to red (fast). The remarkably small range of velocity in this figure was chosen to clarify the following statement: even though all gaps between the cells are equal, water velocity differs. This behaviour correlates to the forces acting on

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**Fig. 3.** The model diatoms (white boxes) are in the equidistant state, i.e. the distances between the single model diatoms are all the same. In this state, the stationary solutions of the computer simulation are velocities—coloured from red (fast) to blue (slow) in a range from 0.1 m s\(^{-1}\) to 0.11 m s\(^{-1}\)—that are not the same in all the gaps between the model diatoms, although the distances are the same. This result is caused by interference phenomena (similar to patterns on a river after a bridge with equidistant pylons).
saling single diatoms. Table 1, which includes diatoms counted from A1 to A10, shows the specific forces acting on each diatom in the x- and y-direction. Note that the ends (A1 and A10) are not the real ends of the chain, because the chain itself has infinite length (periodic boundary conditions). So these ends only build the bounds of an endlessly repeated sequence. To assure the same height of all model diatoms in the simulated chain, the first (A1) and the last (A10) diatom are modelled with half the height (because of the periodic boundary conditions).

The velocity distribution in the gaps shows interferential phenomena (as can be seen from the different sizes of the red coloured areas. The velocities in the gaps between the model diatoms are not equal for every gap even though all the gaps are the same (Fig. 3).

Forces: As can be seen from table 1, the force acting on diatom A1 is positive \(F_{A1} = 830.60 \times 10^{-11} \text{ N}\) and the force acting on diatom A2 is also positive \(F_{A2} = 0.52 \times 10^{-11} \text{ N}\). This means that if the model diatoms were allowed to move freely A1 would move in a positive direction and A2 would also move in a positive direction, but less, because the absolute value of the force is smaller. Therefore, the gap between these two model diatom cells would decrease, since \(F_{A2} - F_{A1} = (0.52 \times 10^{-11} \text{ N} - 830.60 \times 10^{-11} \text{ N})\) gives a negative value for the increase of the gap. The force acting on diatom A3 is negative \(F_{A3} = -5.77 \times 10^{-11} \text{ N}\), and the force on model diatom A4 is positive \(F_{A4} = 1.41 \times 10^{-11} \text{ N}\), and forces the cell into a positive y-direction. Therefore, the gap between these two model diatom cells would increase, since \(F_{A4} - F_{A3}\) gives a positive value. In this way, the changes in gap widths (if the model diatoms were allowed to move) can readily be calculated.

The tendency if one performs these calculations (with data from table 1) is that the single gaps nearly alternately increase and decrease. However, as the simulation shows, attraction and repulsion do not always alternate, but there are some cases where more than two neighboured gaps act the same way: e.g. the gaps A1/A2 and A2/A3 decrease, also the gaps A4/A5 and A5/A6 do not alternate but both increase. The reason for the remarkable

**Tab. 1.** Forces acting on model diatom cells numbered from A1 to A10 for incoming flow conditions of 0.01 m s\(^{-1}\) in the positive x-direction. Due to symmetric boundary conditions the first and the last diatom of the chain (A1 and A10) are only designed half so that forces in the x-direction are also half of the actual value.

<table>
<thead>
<tr>
<th>Diatom</th>
<th>Force (F_{Ai}) in y-direction ([10^{-11} \text{ N}])</th>
<th>Force (F_{Ai}) in x-direction ([10^{-9} \text{ N}])</th>
</tr>
</thead>
<tbody>
<tr>
<td>A1</td>
<td>830.60</td>
<td>12.62</td>
</tr>
<tr>
<td>A2</td>
<td>0.52</td>
<td>25.24</td>
</tr>
<tr>
<td>A3</td>
<td>-5.77</td>
<td>25.24</td>
</tr>
<tr>
<td>A4</td>
<td>1.41</td>
<td>25.24</td>
</tr>
<tr>
<td>A5</td>
<td>3.30</td>
<td>25.24</td>
</tr>
<tr>
<td>A6</td>
<td>3.46</td>
<td>25.24</td>
</tr>
<tr>
<td>A7</td>
<td>1.68</td>
<td>25.24</td>
</tr>
<tr>
<td>A8</td>
<td>-6.10</td>
<td>25.24</td>
</tr>
<tr>
<td>A9</td>
<td>0.59</td>
<td>25.24</td>
</tr>
<tr>
<td>A10</td>
<td>-829.50</td>
<td>12.62</td>
</tr>
</tbody>
</table>
increase of force on A1 and A10 is unknown (Tab. 1). Perfect alternating increase and decrease of neighbouring gaps would represent the highest possible frequency of the oscillatory system the model diatom chain is proposed to be. This leads to the second case investigated, paired model diatoms.

Paired model diatoms: In the second case investigated, the distance between the cells is fixed and alternates between the minimum (10 μm) and the maximum distance (20 μm) the model diatoms can achieve. Again, there is an inlet flow of 0.1 m s\(^{-1}\) in the positive x-direction. Also in this case, interference phenomena in the velocity distribution appear, but this time they are negligible compared to the effect of the velocity in the larger gaps being much larger than the velocity in the smaller gaps (Fig. 4). Therefore the static pressure is much lower in the larger gaps and acting forces tend to readjust the chain into a balanced equidistant state. Table 2 shows the acting forces in two different directions. The alternating algebraic sign for forces directed in the y-direction easily shows the described behaviour, if one performs the calculation for gap-distance as above. The fact that an imbalanced state tends to establish the balanced state is, however, a more effect than the first case investigated.
Discussion

This work is a numerical simulation. Experimental verification of the results is highly desirable. Even though there is a high grade of convergence in the simulations, numerical failure can never be excluded. The following interpretation only refers to the results from the numerical approximations as described above.

The stationary result of the equidistant state forces the chain into imbalance of distance between cells. The stationary result of a non-equidistant state forces the equilibrium as shown in the other exemplary solution. This leads to the conclusion that there may be an additional oscillatory movement to the expected acceleration in the flow direction during the time of relative motion between chain and fluid. It is a behaviour that is comparable to the so-called flutter mechanism in turbine flows (NOWINSKI and PANOVSKY 2000), even though the flutter mechanism is mainly described as an aero-elastic phenomenon and therefore relevant in gas-flows. In the examples described here, it would be an example of hydro-elasticity that is concerned, with the motion of bodies through (BISHOP and PRICE 1979).

The assumption of a diatom colony with exactly the same distance between all neighbouring cells is an idealistic one. In real diatom chains the gaps are not exactly the same, i.e., the chain is imbalanced. According to the computer simulations such a chain aspires to reach the «balanced» configuration with equidistant cells. However, the state with perfectly equidistant cells will never be reached and therefore oscillations occur as long as there is a non-zero relative velocity between the chain and the surrounding fluid. Supposing that the natural habitat of the diatom colony is the open sea with its unsteady flow conditions such relative motion between diatoms and water is likely, and diatoms may have evolved a mechanism to utilize such flow changes, i.e., structure leading to function: oscillatory movement increases the advective diffusion through the surface of the diatoms and therefore increases nutrient supply in a homogeneous nutrient solution (PAHLOW et al. 1997).

Tab. 2. Forces acting on diatoms numbered from A1 to A10 for incoming flow conditions of 0.01 ms^{-1} in the positive x-direction. Due to symmetric boundary conditions, the first and the last diatom of the chain (A1 and A10) are only depicted as halves, so that forces in the x-direction are also half of the actual value.

<table>
<thead>
<tr>
<th>Diatoms</th>
<th>Force in y-direction [10^{-9} N]</th>
<th>Force in x-direction [10^{-9} N]</th>
</tr>
</thead>
<tbody>
<tr>
<td>A1</td>
<td>74.36</td>
<td>22.28</td>
</tr>
<tr>
<td>A2</td>
<td>9.99</td>
<td>50.36</td>
</tr>
<tr>
<td>A3</td>
<td>-9.70</td>
<td>50.46</td>
</tr>
<tr>
<td>A4</td>
<td>10.29</td>
<td>50.44</td>
</tr>
<tr>
<td>A5</td>
<td>-10.34</td>
<td>50.46</td>
</tr>
<tr>
<td>A6</td>
<td>10.26</td>
<td>50.46</td>
</tr>
<tr>
<td>A7</td>
<td>-10.25</td>
<td>50.44</td>
</tr>
<tr>
<td>A8</td>
<td>10.22</td>
<td>50.48</td>
</tr>
<tr>
<td>A9</td>
<td>-10.45</td>
<td>50.39</td>
</tr>
<tr>
<td>A10</td>
<td>-74.46</td>
<td>17.65</td>
</tr>
</tbody>
</table>
The question of how a linked diatom chain gets the signal to build end valves is a question long discussed in the diatom community (e.g. Fryxell 1976, Crawford 1979, Davey and Crawford, 1986, Crawford and Sims, 2007). The computer simulation results presented here indicate various velocities of the water in the gaps and variance in the forces acting on the model diatom cells. This might provide a needed »signal« for building end valves (Kooistra pers. comm.).

A comparison of the results with a turbulent computation with the same boundary conditions shows the same effect but with forces ten times stronger than the laminar solution. The existence of a similar interference in a laminar calculation also shows that the modelled effects are not only turbulence phenomena, but inherently have to do with the inner elasticity of water. More detailed modelling approaches as well as experimental corroboration of the modelling results are needed to verify if real diatom chains exposed to conditions as described above also exhibit the oscillatory movement that results from this modelling study.

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COLONIAL DIATOMS AND OSCILLATORY MOVEMENT