

MICROFLUIDIC SIMULATION OF A COLONIAL DIATOM CHAIN REVEALS OSCILLATORY MOVEMENT

I.C. Gebeshuber

Vienna University of Technology, Institut fuer Allgemeine Physik, Wien, Austria

Vienna University of Technology, TU BIONIK Center of Excellence for Biomimetics, Wien, Austria

AC²T Austrian Center of Competence for Tribology, Wiener Neustadt, Austria

ille@iap.tuwien.ac.at

J. Srajer

Vienna University of Technology, Institut fuer Allgemeine Physik, Wien, Austria

Vienna University of Technology, TU BIONIK Center of Excellence for Biomimetics, Wien, Austria

e0326080@student.tuwien.ac.at

1 Introduction

Diatoms are single-celled organisms with rigid parts in relative motion at the micro- and nanometer length scales. This makes them interesting for nano- and microtechnological applications [1-6]. Some diatom species form colonies comprising many cells in form of long chains [7]. *Rutilaria philipinnarum* is an example of such a species. *R. philipinnarum* is a fossil colonial diatom thought to have lived in inshore marine waters [8]. In this species, the single diatoms connect by linking spines and by a complex siliceous structure termed the periplekton what can be seen in a simple drawing in Figure 1. The spines are arranged in an elliptic way around the periplekton in the middle. On one hand these structures keep the cells together, but on the other hand also keep distance between the cells so that there is still some fluid between the cells. Hence the shape of the spines allows expansion of the chain to a certain maximum length and compression to a minimum [4].

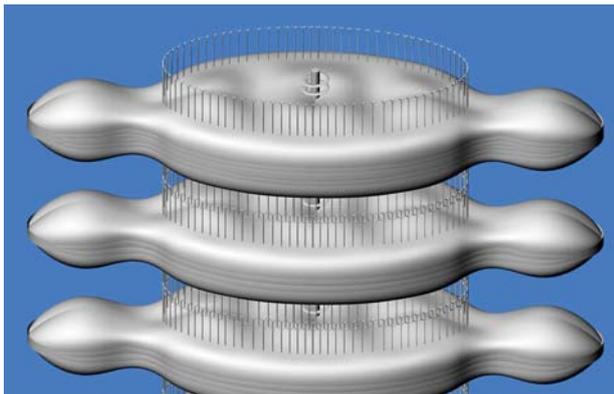


Figure 1: A schematic drawing of the linking structures of *R. philipinnarum* is shown. On top of the last diatom the periplekton in the center of the diatom-body and ring-like arranged long spines are illustrated. They are supposed to keep distance between the cells in a variable way between a minimum and maximum distance.

Such elaborated linking mechanisms as shown in a schematic drawing in Figure 1, inspired the question what would happen to such a diatom colony subjected to water flow. A diatom chain subjected to fluid flow is soon being moved as a whole with the flow. 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 that situation of acceleration, water flows through the gaps between the single cells creating relative motion between the chain and water.

To analyze the problem, the method of Computational Fluid Dynamics (CFD) is used. CFD is one of the branches of fluid mechanics that uses numerical methods 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 [9]. Indeed, these equations are so closely coupled and difficult to solve that it was not until the advent of modern computers in the 1960s and 1970s that they could be resolved for real flow problems within reasonable timescales. A basic introduction to fluid mechanics for the interested reader is given by CHORIN and MARS DEN [10]. Numerical methods used to solve the governing equations in fluid mechanics can be found in LEVEQUE [11].

The computer simulations presented here shall inspire biologists working on diatoms to perform experiments validating the results, and thereby initiate interdisciplinary research involving groups from technical and biological backgrounds [12].

2 Materials and Methods

As a basic start to prove the principle a simple two-dimensional finite element model of a diatom chain was created. This model chain does not contain linking spines or periplekton or exact surface conditions of the diatoms, but solely concentrates on primary aspects concerning the boundary conditions of multiple gaps. The problem investigated here has remote similarity to the circumfluence of the river Thames on the pylons of the medieval London Bridge (Figure 2).

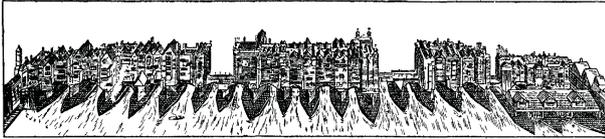


Figure 2: Medieval London Bridge. Copyright free material from http://www.gutenberg.org/files/19699/19699-h/images/bridges_6.png

Of course the length scale clearly differs: the diatom cell size is assumed to be $140\ \mu\text{m} * 34\ \mu\text{m}$, and that the distance between the cells can achieve a value from $10\ \mu\text{m}$ to $20\ \mu\text{m}$. The colony is assumed to be comprised of single units of 10 cells each that are repeated endlessly. This simplifies calculations on the one side and on the other neglects the influence of the ends of the chain completely

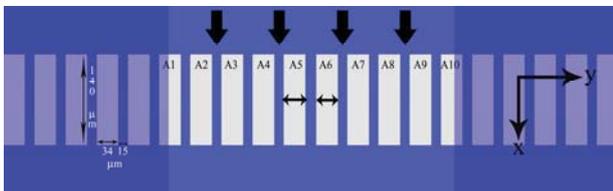


Figure 3: The white boxes counted from A1 to A10 symbolize the model diatoms. The model diatoms have one degree of freedom of movement, namely in $\pm y$ direction, indicated by the arrows in cells A5 and A6. The x - and y -axes of the coordinate system used are given on the right. The size of each model diatom cell is $140\ \mu\text{m} * 34\ \mu\text{m}$, the distance between them is $15\ \mu\text{m}$. 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.

The chain of model-diatoms is surrounded by water. In this simple isothermal model (i.e. no temperature change takes place), undisturbed fluid flow is allowed for between the single cells. The cells do not move actively, and are solely moved by the water. Fluid flow models need inlet and outlet conditions. The inlet fluid velocity is assumed to be from $0.01\ \text{m/s}$ to $1\ \text{m/s}$, what was varied in decimal powers. Because the quality of the results does not change for the range of velocities only the result for $0.1\ \text{m/s}$ is presented here. As an outlet condition an averaged static pressure of one bar is assumed, because the diatoms live near the ocean surface. The Reynolds number (Re) is a dimensionless number that gives a measure of the ratio of inertial forces to viscous forces and quantifies the relative importance of these two types of forces for given flow conditions [13]. The Reynolds number can be written as $Re = \rho * v * L / \eta$, with ρ the density ($\sim 1000\ \text{kg/m}^3$), the velocity v (max. $1\ \text{m/s}$) and η the dynamic viscosity ($1518\ \mu\text{Pa/s}$) of the fluid whereas L is a characteristic length and assumed to be the length of a diatom ($L = 140\ \mu\text{m}$). Reynolds numbers are also used to

characterise two different flow regimes: laminar or turbulent flow. The laminar flow occurs at low Reynolds numbers with $Re < 2300$, where viscous forces are dominant. Turbulent flow occurs at high Reynolds numbers $Re > 2300$ and is dominated by inertial forces, which tend to produce random eddies, vortices and other flow fluctuations [14]. Because of the small scales of the Diatoms the Reynolds numbers for such problems are very low for a wide range of flow conditions and therefore the fluid is characterised by a laminar behaviour.

For solving this boundary value problem the software package ANSYS CFX 11.0 is used. As with various other commercial software packages it uses the finite-volume-method, a standard technique where the equations are solved on discrete control volumes. The models consist of up to 308283 volumes. This mesh of elements was created in ANSYS ICEM CFD 11.0.

3 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 (see Figure 3). There are also two different possible directions of the fluid to flow: along the long axis of the chain in y -direction or across the chain through the gaps in 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 is not 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, Figure 4). 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_{\min} between A1 and A2, d_{\max} between A2 and A3, d_{\min} between A3 and A4, d_{\max} between A4 and A5, and so on, with d_{\min} being $10\ \mu\text{m}$ and being d_{\max} $20\ \mu\text{m}$). This arrangement is one single example for an imbalanced condition of the chain and is shown in Figure 5. The resulting acting forces grow proportionally with the velocity but do not change in direction with the different velocities investigated ($0.01\ \text{m/s} - 1\ \text{m/s}$). 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 flow direction (x -direction, see Fig. 3) are about a hundred times larger than the forces orthogonal to the flow direction (y -direction, see Fig. 3) for the equidistant state, mainly results for the forces orthogonal to the flow direction are presented. The reason for this is that the solution for the forces in x -direction is trivial: the whole chain of model diatoms accelerates in the direction of the flow.

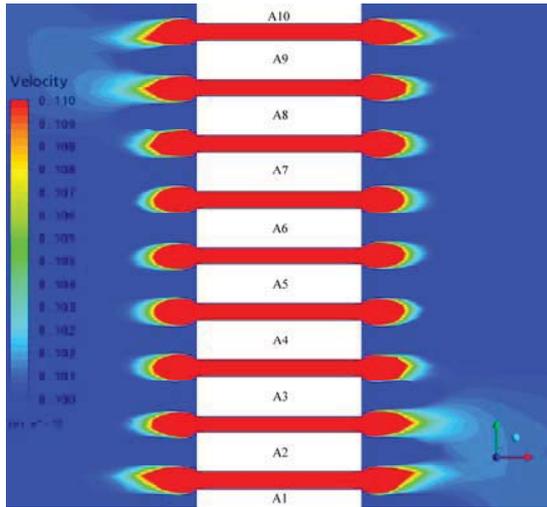


Figure 4: The model diatoms (white boxes) are in the equidistant state, i.e. the distances between the single model diatoms are all the same. In this state, the stationary solutions of the computer simulation are velocities - coloured from red (fast) to blue (slow) in a range from 0.1 m/s to 0.11 m/s - 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).

Forces on the cells strongly correlate with the static pressure of the surrounding fluid, which again corresponds to the surrounding fluid velocity. For inviscid fluids Bernoulli's principle states that an increase in speed of the fluid occurs simultaneously with a decrease in pressure [14].

3.1 Equidistant model diatoms

Figure 4 shows the result for an inlet flow-velocity of 0.1 m/s in 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 (see Figure 4). This behaviour correlates to the forces acting on single diatoms (see Table 1), which includes diatoms counted from A1 to A10 shows the specific forces acting on each diatom in x- and y-direction. Note that the ends (A1 and A10) are not the real end 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 (see Figure 4).

Table 1: Forces acting on model diatom cells numbered from A1 to A10 for incoming flow conditions of 0.01 m/s in 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 x-direction are also half of the actual value

Diatoms	Force F_{Ai} in y-direction [10^{-11} N]	Force F_{Aj} in x-direction [10^{-9} N]
A1	830.60	12.62
A2	0.52	25.24
A3	-5.77	25.24
A4	1.41	25.24
A5	3.30	25.24
A6	3.46	25.24
A7	1.68	25.24
A8	-6.10	25.24
A9	0.59	25.24
A10	-829.50	12.62

Forces: As can be seen from Table 1, the force acting on diatom A1 is positive ($F_{A1} = 830.60 \cdot 10^{-11}$ N) and the force acting on diatom A2 is also positive ($F_{A2} = 0.52 \cdot 10^{-11}$ N). This means that – if the model diatoms were allowed to move freely – A1 would move in positive direction and A2 would move – but less, because the absolute value of the force is smaller – also in positive direction. Therefore, the gap between these two model diatom cells would decrease, since $F_{A2} - F_{A1}$ ($0.52 \cdot 10^{-11}$ N - ($830.60 \cdot 10^{-11}$ N)) gives a negative value for the increase of the gap. The force acting on diatom A3 is negative ($F_{A3} = -5.77 \cdot 10^{-11}$ N), and the force on model diatom A4 is positive ($F_{A4} = 1.41 \cdot 10^{-11}$ N), and forces the cell into 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 freely) 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 neighbored 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 increase of force on A1 and A10 is unknown (see Table 1). Perfect alternating increase and decrease of neighbored gaps would represent the highest possible frequency of an oscillatory system, as it is proposed to be. This special behaviour of the chain, that a distance balanced state want to become unbalanced, was not expected. This leads to the second case investigated, paired model diatoms.

3.2 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) our model diatoms can achieve. Again, there is an inlet flow of 0.1 m/s 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 that the velocity in the larger gaps is much faster than the velocity in the smaller gaps (see Figure 5).

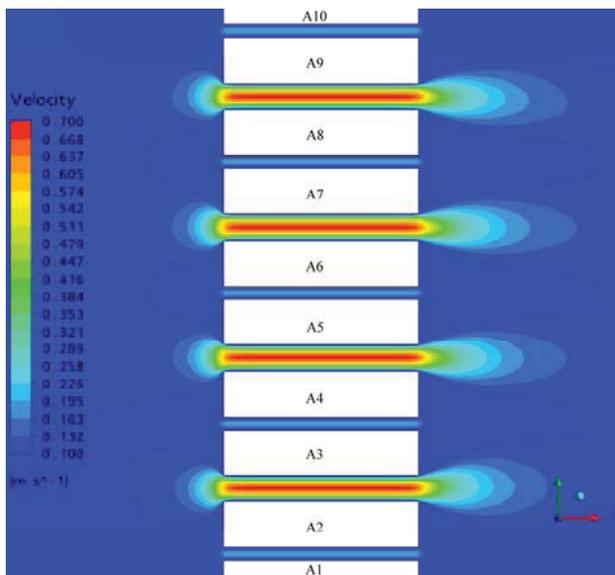


Figure 5: The model diatoms (white boxes) are in the paired state, i.e. the distances between two model diatoms are fixed and are alternately small or large. A stationary solution of the computer simulation is calculated. Velocity - coloured from red (fast) to blue (slow) in a range from 0.1 m/s to 0.7 m/s - is distinctively larger in the large gaps compared to the velocity in the small gaps. This velocity distribution leads to higher static pressures in the small gaps. Furthermore, the cells are forced to reduce the distance of the larger gaps while enlarging the smaller ones.

Therefore the static pressure is much lower in the larger gaps and acting forces tend to readjust the chain into balanced equidistant state. Table 2 shows the acting forces again in two different directions. The alternating algebraic sign for forces directed in 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 conceivable effect than the first case investigated

4 Conclusions, Discussion and Outlook

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 into the equilibrium again as shown in the second exemplary solution.

Table 2: Forces acting on diatoms numbered from A1 to A10 for incoming flow conditions of 0.01 m/s in 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 x-direction are also half of the actual value.

Diatoms	Force in y-direction [10^{-9} N]	Force in x-direction [10^{-9} N]
A1	74.36	22.28
A2	9.99	50.36
A3	-9.70	50.46
A4	10.29	50.44
A5	-10.34	50.46
A6	10.26	50.46
A7	-10.25	50.44
A8	10.22	50.48
A9	-10.45	50.39
A10	-74.46	17.65

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 [15], 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 hydroelasticity that is concerned with the motion of deformable bodies through liquids [16]. Oscillatory movement increases the advective diffusion through the surface of the diatoms and therefore increases nutrient supply in a homogeneous nutrient solution [17].

The question how a linked diatom chain gets the signal to build end valves is a question long discussed in the diatom community [18-21]. 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. 2008).

A comparison of these results with a non-turbulent (laminar) solution with the same boundary conditions shows the same effect but with forces a tenth of the strength as when using the k- ϵ -turbulence method. This leads to the proposition that turbulence modelling plays a mayor role for solving such problems close to reality. 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 inner elastics 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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