"S.o.f.t": Swimmers, one few, thousands

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Unicellular swimmers, e.g., *E. coli* bacteria, spermatozoa, or paramecia are typically of a few micrometers in size and their swimming velocities are of the order of one body length per second. At these scales, viscous damping by far dominates over inertia, and the physics of their swimming is very different from that applying to swimming in the macro-world. While inertia is the dominant propulsion mechanism for swimming in the macro-world, microorganisms use the viscous drag of the surrounding fluid for their propulsion. Spawned by the non-trivial nature of this viscosity-based swimming and its important applications in biology, the study of the fundamental physics of microswimmers has become an active field of research during the past 30 years.

In nature, swimmers never swim alone. Coordinated motion is exploited by spermatozoa, which self-assemble to increase motility. Bacteria grow by dividing and collectively invading their surroundings. Assemblies of motile microorganisms, exhibit highly organized movements with remarkable large-scale patterns such as networks, complex vortices, or swarms. Understanding, and controlling the emergent collective behaviour has therefore become an important challenge. To this aim, artificial microswimmers have been produced, that could mimic the behaviour of biological ones. Artificial microswimmers also have a high potential for biomedical and technological applications, as they could be used for targeted drug delivery or to modify the properties of the liquid where they are introduced (e.g. viscosity). Several kinds of artificial microswimmers have been produced so far, based on different mechanisms, among which artificial flagella activated by external magnetic fields, chemical reactions, ejection of nanobubble.

In the first part of the project, we addressed the study of a novel kind of artificial microswimmer developed at the MPI-DS in the last years, consisting of self-propelled liquid droplets driven by the so-called Marangoni flow. This system exploits the concept of surface tension, a tangential force originating at the interface between two different phases (e.g. oil and water). Some substances (surfactants) have a tendency to migrate towards interfaces, lowering their surface tension. A typical example is soap. These novel microswimmers consist of an emulsion of liquid droplets immersed in a second immiscible liquid. A non-uniform surface tension distribution is created on the droplets' surface, through a non-uniform distribution of surfactants. This creates a net tangential force at the surface (Marangoni stress), which sets a convective motion both inside and outside the droplet. Hence, propulsion arises due to momentum conservation (Fig.1.a). Surface tension gradients can originates, e.g. from chemical reactions changing the surfactant structure - Belousov-Zhabotinsky (BZ) reactions- or (b) by phase separation phenomena in non-equilibrium conditions - liquid crystal droplets, immersed in a solution of water/ionic surfactant. The purpose of our study was a detailed investigation of the propulsion mechanism of these droplets and its dependence on the experimentally tuneable parameters, such as the size of the droplets and the surfactant concentration. To this aim, we developed a flexible numerical model, based on a method that allows to track the position of a moving and deformable interface (level set method), easily adaptable to different kinds of swimmers. In our treatment we take into account the influence that the flow has
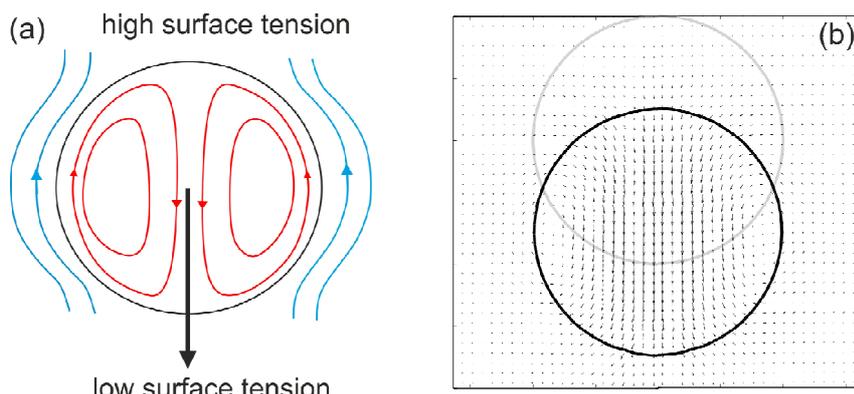

FIGURE 1.
(a) Schematic representation of an active droplet driven by Marangoni flow and (b) its velocity field (arrows) as derived from level-set simulations (grey: initial position of the droplet, black: after some time)

FIGURE 2.
Formation of chemotactic band
(a) Experiments: the white thick
line is the border of the bubble,
the small dots are bacterial
(b) Simulations: d is the distance
from the bubble interface, S/S₀ is
the bacterial concentration at
different times, normalized with
the initial one
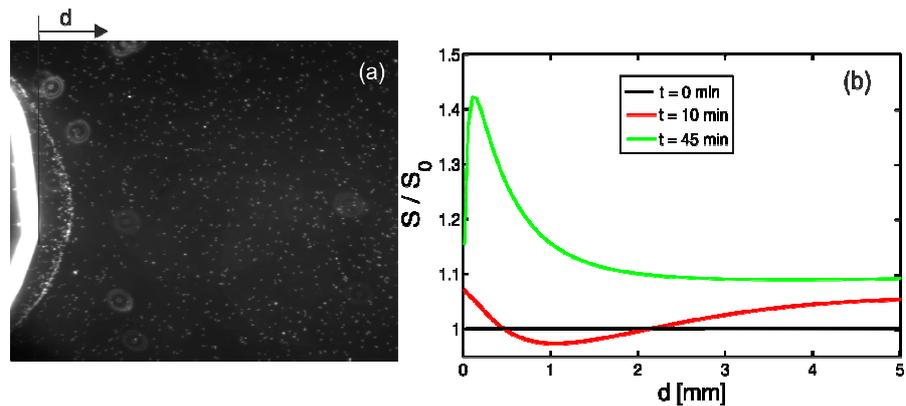
on the motion of microswimmers and vice-versa: we solve the momentum equation for the fluid (Navier-Stokes equation), thus deriving the velocity field inside and outside individual droplets. We also account for mass transport phenomena (surfactant diffusion) both on the droplet's surface and in the surrounding liquid, adsorption/desorption processes at the surface and chemical reactions depleting the surfactant. The model was validated by comparison with the analytical solution for selected scenarios. It was then adapted to study the kinds microswimmers mentioned above. The numerical simulations reproduced several propulsion mechanisms observed in experiments, such as the insurgence of a self-sustained motion in a BZ reaction droplet, as a consequence of an initial random displacement. Interestingly, they also reproduced a typical chemotactic behaviour, i.e. the motion of a microswimmer as a response to a gradient, such as a gradient of surfactant concentration in the liquid, in the direction of the maximum concentration (Fig. 1.b). This behaviour has been observed experimentally at the MPI-DS, for both artificial and biological microswimmers. For bacteria it has a particular relevance, as it drives their motion in the quest for nutrients and substances required for their respiration. These results will provide the background to target the design of microswimmers for medical applications such as localized drug deliver, as the model can be easily extended to account for a 'cargo' inside the droplets (a liquid of a different density).

In the second part of the project we addressed the collective behaviour of biological microswimmers performing chemotaxis. In particular we considered a system with a great technological potential for the production of bio-fuel, the *Shewanella Oneidensis* bacteria. These bacteria are endowed with tubular structures (similar to micro-cables), used to shift electrons towards an electron acceptor (e.g. metals or oxygen), during their respiration process. They can live both in aerobic and anaerobic conditions and are commonly found in water. They tend to aggregate around minerals, creating a denser area (chemotactic band), precursor for a biofilm. This biofilm could be exploited to produce energy (it acts like a micro-battery) as well as to reduce metals for chemical purposes. However, the time required to form these aggregates (several days) constitutes a significant limitation. Recent experiments performed at the MPI-DS, showed that a similar behaviour is also triggered by the proximity to an air bubble. In this case the *Shewanella* collect around the bubble forming a chemotactic band, within one to few hours (Fig.2). The purpose of our study was to investigate this mechanism and assess the parameters influencing the formation time of the chemotactic band, e.g. the bubble size and the initial bacterial concentration . The ultimate goal was to find a way to minimize the formation time. To this aim, we developed a numerical model, tracking the time evolution of the concentration fields of Shewanella. The model accounts for the air diffusing from the bubble into the surrounding water, the consequent shrinking of the bubble, the chemotactic behaviour of the bacteria , their random mobility and their reproduction. The numerical results (Fig 2.b) were in line with the experimental one (Fig. 2.a), both qualitatively and quantitatively. We developed a parametric study, finding the optimal conditions to minimize the band formation time. We also added an acoustic driving to the bubble (time-periodic pressure wave), finding that the formation time of the chemotactic band was reduced to few minutes. This prediction will have to be verified by experiments, as it has a vast technological potential.