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Numerical simulation of artificial microswimmers driven by Marangoni flow

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ABSTRACT

In the present paper the behavior of a single artificial microswimmer is addressed, namely an active droplet moving by Marangoni flow. We provide a numerical treatment for the main factors playing a role in real systems, such as advection, diffusion and the presence of chemical species with different behaviors. The flow field inside and outside the droplet is modeled to account for the two-way coupling between the surrounding fluid and the motion of the swimmer. Mass diffusion is also taken into account. In particular, we consider two concentration fields: the surfactant concentration in the bulk, i.e. in the liquid surrounding the droplet, and the surfactant concentration on the surface. The latter is related to the local surface tension, through an equation of state (Langmuir equation). We examine different interaction mechanisms between the bulk and the surface concentration fields, namely the case of insoluble surfactants attached to the surface (no exchange between the bulk and the surface) and soluble surfactants with adsorption/desorption at the surface. We also consider the case where the bulk concentration field is in equilibrium with the content of the droplet. The numerical results are validated through comparison with analytical calculations. We show that our model can reproduce the typical pusher/puller behavior presented by squirmers. It is also able to capture the self-propulsion mechanism of droplets driven by Belousov–Zhabotinsky (BZ) reactions, as well as a typical chemotactic behavior.

1. Introduction

Unicellular swimmers, e.g., E. coli bacteria, spermatozoa, or paramecia are typically of a few to several ten micrometers in size and their swimming velocities are of the order of one body length per second. Due to their small size and swimming velocities, the Reynolds number of the flow involved in their swimming is much smaller than unity. As a consequence, viscous damping by far dominates over inertia, and the physics ruling their swimming is very different from that applying to swimming in the macro-world [1–3]. While inertia is the dominant propulsion mechanism for swimming in the macro-world, microorganisms make use of the viscous drag of the surrounding fluid for their propulsion. Initiated by the non-trivial nature of viscosity-based swimming and its important applications in biology, the study of the fundamental physics of swimming at low Reynolds numbers has become an active field of research during the past 40 years [1,4–7].

Several kinds of artificial microswimmers have been produced, based on different mechanisms [8,9], with a potential for technological applications such as targeted drug delivery, removal of pollutants, waste treatment. Examples of artificial

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microswimmers consist in active liquid droplets immersed in a second immiscible liquid and propelled by Marangoni flow. The underlying idea is to create a non-uniform surface tension distribution on the droplet surface, through a non-uniform distribution of surfactants, i.e. molecules of a third kind dissolved inside the solution and migrating to the surface [10]. To satisfy the local balance of forces at the interface, a Marangoni stress originates, tangent to the surface, from the area with a lower surface tension to the one with a higher surface tension. From this, a convective fluid motion is set inside and outside the droplet and, therefore the droplet starts moving.

Such surface tension gradients can arise (a) from chemical reactions changing either the structure of the surfactant molecules [11–14] or the surfactant coverage [15,16] as well as (b) by dissolution or phase separation phenomena under non-equilibrium conditions [17,18]. Intriguing systems have been produced, based on such principles, such as self-propelled droplets driven by Belousov–Zhabotinsky (BZ) reactions [19,20], behaving like non-equilibrium chemical oscillators. Some experiments showed that nematic liquid crystal droplets, immersed in a solution of water/ionic surfactant, can develop spontaneous motion [21]. Also in this case, the propulsion mechanism appears to be a Marangoni flow, originating from a combined effect of the surfactants and the liquid crystals (i.e. non-isotropic molecules) perpendicularly anchoring to the surface. The details of this mechanism are still unknown.

Active droplets moving by Marangoni flow can be considered “squirmers”, i.e. swimmers where a tangential velocity of the surface drives propulsion. Theoretical works on this class of swimmers have investigated the velocity field generated by individual squirmers [22,23], their hydrodynamic interactions [24,25], and the resulting collective behavior [26]. The majority of this works assumes a prescribed fluid flow at the surface, instead of deriving it. However, for self-propelled droplets driven by gradients of mass concentration or temperature [27,28] or by Belousov–Zhabotinsky (BZ) reactions [19], as well as for emulsion droplets [29,30] of the kind described in [21], analytical solutions of the flow profiles are available for simplified cases, and the stability analysis of their motion has been addressed [31–35].

The description of more realistic scenarios requires to account for a large number of factors, such as the two-way coupling between the flow and the active droplet, several mutually interacting chemical species, mass exchanges between the droplet’s interface and the surrounding liquid (bulk), chemical reactions. In such cases, the numerical approach can be a powerful instrument to investigate the problem at hand.

Several numerical techniques have been developed during the last decades, to track the motion of interfaces: (i) “interface tracking methods”, where the displacement of the interface is tracked in a direct-fashion, e.g. through a set of Lagrangian marker points located on the surface itself (front-tracking [36]); (ii) “interface capturing methods”, where the motion of the interface is described in an implicit-fashion, by following the evolution of an additional function; examples are: immersed boundary [37], finite elements (FEM) [38], volume of fluid (VOF) [39], marker-and-cell [40], level set [41,42] and hybrid methods such as VOF/level set [43]. Combined approaches between (i) and (ii) have also been adopted in order to simultaneously address the interface motion, the flow field around the interface and the surfactant diffusion on the surface. For instance, Lagrangian points marking the interface have been used in combination with a finite difference method for the evolution of the surfactant distribution on the interface and a boundary integral method for the Stokes equations in the fluid [44]. In the present paper, we use a level set approach [45–48] with a continuous surface force formulation [49], in combination with a flow solver based on a projection method [50] to track the motion of the fluid both inside and around the droplet. A vast literature is available for level set methods, including some books [46,48]. For a review, we refer the reader to Ref. [47]. Level set methods have proven particularly efficient when singularities and disconnected bodies are present [51–53]. They allow for the treatment of deformable droplets as well as for a straightforward extension to the case of multiple swimmers. Several authors have numerically studied biphasic systems with surfactants using different methods: arbitrary Lagrangian–Eulerian [43], VOF [39], finite difference/front-tracking [54–57], the diffuse-interface or phase-field method [58]. However, to our knowledge, only few have made use of a level-set formulation, to address the case of insoluble surfactants [41,59–61].

The aim of the present work is to provide a numerical model that could be adapted to the study of real artificial microswimmers moving by Marangoni flow, such as BZ-reaction driven droplets [19,20,35] and emulsion droplets of the kind described in [21]. The description of these systems requires to account for the two-way coupling between the droplet’s motion and the fluid flow, as well as multiple mutually interacting concentration fields (e.g.: empty micelles, filled micelles, liquid crystals, molecular surfactant [21,29]). We wish to provide here a numerical treatment for the main phenomena playing a role in such systems: the flow field, the surfactant advection and diffusion, both in the liquid bulk and on the surface of the droplet, as well as the interaction between the bulk and the surface (adsorption/desorption). The case where a concentration field dissolved inside the bulk is in equilibrium conditions with a droplet of the same substance (e.g. liquid crystals in the emulsion droplets of [21]) is also addressed.

In Fig. 1 we display a simplified sketch of a possible scenario addressed by our code, where an active droplet moves by Marangoni flow. A surfactant concentration field is present, both on the surface of the droplet Γ and in the bulk c. The non-uniform surface concentration induces a non-uniform surface tension field on the surface. In particular, a higher concentration of surfactant corresponds to a lower surface tension, since the surfactants produce a local ‘weakness’ at the interface. Through a local force balance, one can see that a tangential flow originates at the interface – see gray lines (red and light-blue online) – both inside (red online) and outside the droplet (light blue online). By momentum conservation, the droplet moves in the direction indicated by the thick black arrow. The presence of surfactant concentration fields only outside the droplet and on the surface yields the one-sided nature of the problem. Based on embedded finite difference schemes, our work presents a novel treatment of such a situation.