NUMERICAL MODELLING OF THERMOCAPILLARY FLOW ON SUPERHYDROPHOBIC SURFACES

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ABSTRACT
A liquid in Cassie-Baxter state confined between two microstructured superhydrophobic surfaces has a large free surface fraction while at the same time being in close contact to a solid. As such this configuration is predestined for thermocapillary transport when applying a temperature gradient along the structured substrate. We numerically investigate thermocapillary flow over superhydrophobic arrays of fins. Since even moderate temperature gradients of the order of a few K/cm can induce flow velocities of several mm/s, this setup lends itself for microfluidic pumping. We compare the numerical results to an analytical expression for the flow velocity obtained in the limit of Stokes flow.

KEYWORDS: Thermocapillary Flow, Superhydrophobic Surfaces, Microfluidic Pumping

INTRODUCTION
The ability to pump fluid is essential for most microfluidic applications. Usually this is achieved by pressure driven flow or electroosmotic pumping. Generally this needs moving parts or is difficult to miniaturise. An alternative is using surface tension forces for actuation in the form of capillary rise for filling a channel. However, no continuous pumping can be achieved in this way. In this paper we present a means for fluid actuation using thermocapillary flow on superhydrophobic surfaces, where the liquid is in a Cassie-Baxter state confined between two microstructured surfaces with a temperature gradient applied along the structured substrate. Due to the large free surface fraction, even moderate temperature gradients of the order of a few K/cm can induce flow velocities of several mm/s, making this setup suitable for microfluidic pumping. The numerical results are compared to an analytical expression for the flow velocity obtained in the limit of Stokes flow. We note that the considered scenario is different from the thermocapillary motion of liquid drops on fibers, surfaces or in channels reported so far.

THEORY
In our model system the liquid is assumed to be water in a Cassie-Baxter state above a finned surface. A temperature gradient is applied perpendicular to the fin structure (figure 1). At the gas-liquid interface Marangoni stresses exert a force on the liquid driving it towards the regions of higher surface tension while the shear stress in the gas is assumed to vanish. At the fin surfaces a no-slip boundary condition is assumed. As sketched in figure 1, this leads to a spatially varying near-wall flow profile extending a distance of the order of the fin spacing, 2L, into the liquid, while a plug flow of velocity \( u_{th} \) prevails in the bulk of the liquid.

![Figure 1: Sketch of the geometry; left: macroscopic view, right: magnification of the near wall region. In this example we assume a temperature gradient perpendicular to the fins. The gas-liquid interface is assumed to be flat. Apart from a region close to the wall, the velocity field can be approximated as a plug flow.](image)

We model this system by solving the coupled Navier-Stokes and heat transport equations

\[
\rho (u \cdot \nabla)u = \eta \Delta u - \nabla p, \quad \nabla \cdot u = 0
\]

and

\[
(u \cdot \nabla)T = D_T \Delta T
\]

via the finite-element method using Comsol multiphysics. Here \( u, p \) and \( T \) are the velocity, pressure and temperature fields respectively, while \( \rho, \eta \) and \( D_T \) are the fluid’s density, viscosity and thermal diffusion coefficient. Due to the symmetry of the problem it suffices to consider a rectangular domain extending between two fin centers and applying periodic boundary conditions in the direction of the flow, i.e. \( u(x + 2L, y) = u(x, y), \) \( p(x + 2L, y) = p(x, y) \) and \( T(x + 2L, y) = T(x, y) + 2L \frac{\Delta T}{T} \), with \( \frac{\Delta T}{T} \) being the applied temperature gradient at the substrate. Our analysis focuses on substrates of high thermal conductivity such as silicon and thus assumes the temperature at the fin surface to be fixed by the externally applied temperature gradient. In particular, since the fins are assumed to have a large aspect ratio, the temperature at the fin surface in contact with the water is assumed to be constant on each fin and varying by \( 2L \frac{\Delta T}{T} \) from fin
to fin. The gas-liquid interface is approximated as being adiabatic. The velocity boundary condition at this interface becomes \( \eta \partial_y u \big|_{y=0} = (\partial\sigma/\partial T) \partial_y T \), where \( \sigma \) is the surface tension. In the center of the channel at \( y = D/2 \) symmetry boundary conditions apply both to the velocity and temperature fields.

**RESULTS AND DISCUSSION**

Figure 2 shows the computed velocity fields, streamlines and temperature profiles for two different applied temperature gradients of 6 K/cm and 19 K/cm. The convective-diffusive transport of heat results in a complex non-monotonic temperature profile along the gas-liquid interface, inducing extended recirculation zones in the case of the large temperature gradient. However, at a distance away from the surface of the order of the fin spacing the flow profile is essentially a plug flow with velocity 1.7 mm/s and 3.2 mm/s, respectively. In [2] an upper bound for this bulk flow velocity was obtained analytically. In the present case these bounds become 1.7 mm/s and 5.4 mm/s, respectively. This bound is thus closely approached for moderate temperature gradients, while the complex flow profile obtained for large temperature gradients strongly reduces the flow rate compared to the ideal case. Nevertheless, the results indicate that thermocapillary convection may even enable larger flow velocities than typically achieved with electroosmosis and may therefore qualify as a versatile pumping principle in microfluidics.

**Figure 2:** Computed velocity field (arrows), streamlines and temperature profile for applied temperature gradients perpendicular to the fin structure of 6 K/cm (left) and 19 K/cm (right). The computational domain extends between two adjacent fin centres, \( 2L = 100 \mu m \), and the free surface fraction is \( a = B/L = 0.8 \) (cf. figure 1). The separation between the two parallel superhydrophobic surfaces is \( D = 400 \mu m \). The model parameters are (assuming water as the liquid): viscosity \( \eta = 1 \text{ mPa s} \), density \( \rho = 1000 \text{ kg/m}^3 \), \( \partial\sigma/\partial T = -0.1514 \text{ mPa m/K} \), thermal diffusivity \( D_T = 0.14 \text{ mm}^2/\text{s} \).

We note that the arrangement with a temperature profile applied perpendicular to the fin structure is not the optimal one. Indeed, as was shown in [2], the velocities achievable when applying the temperature gradient in parallel to the fin structure are generally more than a factor two larger. This is in part due to the analogy of the present situation with pressure driven flow over such surfaces, where the slip coefficient for flow parallel to the structure is exactly a factor 2 larger than for flow perpendicular to it [7]. However, another important factor is highlighted by the present investigation, namely the occurrence of a recirculation in flow direction due to the non-monotonic temperature profile along the gas-liquid interface. In the case of a temperature gradient applied in parallel with the fin structure these rolls are absent due to the symmetry and are instead replaced by counterrotating pairs of rolls perpendicular to the main flow which affects the main flow much less.

**CONCLUSION**

We have numerically investigated thermocapillary flow of a liquid in Cassie-Baxter state confined between two microstructured superhydrophobic surfaces. In particular, the flow over superhydrophobic arrays of fins with a temperature profile applied perpendicular to the fin surface was investigated. The presented results compare favorably to an analytical expression for the flow velocity obtained in the limit of Stokes flow [2], at least for small temperature gradients, but also highlight the fact that recirculation rolls due to the complex temperature profile at the liquid-gas surface averting achieving the full potential for actuation in this particular configuration. Nevertheless, even moderate temperature gradients of the order of a few K/cm can induce flow velocities of several mm/s, compatible with velocities realized in microfluidic settings by electroosmotic or pressure driven pumping.

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