Using CFD to study the effect of contact angle on microdroplet deformation

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In this paper we present computational fluid dynamics (CFD) simulation results that demonstrate the effect of surface hydrophobicity on the deformation of a droplet moving through a contraction in a microchannel. A commercial package CFD-ACE+ (CFDRC, www.cfdrc.com) with a volume of fluid code (VOF) was used, and the code was validated against experimental data, and against another VOF code, MAC2 (Rudman, International Journal of Numerical Methods, 98).

Depending on the conditions, a droplet that is initially larger than a contraction can either follow the streamlines and stretch to a tube shape inside the contraction due to the domination of viscous forces, or alternatively, surface tension can pull the droplet together to form slug flow in the contraction. The capillary number, which indicates the ratio of the viscous force to the surface tension force, scales with the droplet diameter. Thus, as droplet shape and deformation in microchannels are generally dominated by surface tension, the droplets will often fill the contraction. This phenomena means that the droplet liquid interacts with the channel surface in the contraction, which makes surface-property induced shape manipulation possible.

Even though hydrophobic surface forces act over distances less than 100nm (see Israelachvili's book 'Intermolecular and Surface forces') the CFD code is able to predict the bulk effect of the contact angle via varying the interface normal with the contact angle. We have demonstrated how surface patterning techniques can be exploited to help control the deformation and breakup of droplets, and show examples where early breakup and the formation of controlled satellite droplets can be achieved.