Dynamics of a Sessile Droplet Evaporation

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Abstract

Evaporation of sessile droplets is associated with simple phenomena such as the ring-like spot left by a drying coffee droplet. Accardo A. et al. [1] found that evaporation rate plays an important role on the convective motion inside the droplet that are responsible of amyloid β-type fiber aggregates of proteins which are very important in the study of degenerative diseases such as Alzheimer [2]. Here the evaporation of a sessile droplet with a pinned contact line was investigated by COMSOL and MATLAB®. Since the evaporation is very slow respect to the time the aqueous vapor concentration adjusts, the evaporation was considered a quasi-steady-state process (Second Fick's Law). Hence, the vapor concentration distribution above the droplet satisfied the Laplace equation but with a time-varying droplet surface [3]. It was supposed that the net evaporation rate from the droplet remains almost constant with time, even though the evaporation flux becomes greater at the edge of droplet rather than in the central part (see Figure 1a). Another initial hypothesis is that the contact angle in correspondence of which the contact interface starts to recede is about 4° on poly metil methachrylate (PMMA) flat substrate; the final step of the simulation is conducted until this value because the free surface becomes inhomogeneous with this model afterwards (Figure 1d). The shrinkage evolution was obtained both in MATLAB® through an in-house code and COMSOL. In both cases a spherical cap profile starting from an initial contact angle of 40° (Figure 1b) was considered. In the first case, the new contact angle at the time (t+1) was obtained from the difference between the water volume at time t and the lost mass due to evaporation at (t+1). Since the free surface can be described by the sphere equation, the condition of pinned interface and the new contact angle allowed to plot the dynamics at each step (Figure 1c). In the second case, the axysimmetry geometry and the moving mesh (Arbitrary Langrangian-Eulerian Method) were used. The downward movement of the free surface was given by dividing the evaporation rate by the density. A further step will be to integrate this model with the fluid dynamic inside the droplet in order to compute the inner convective motions. In particular, detailed simulations are required to optimize the experimental set-up of an evaporation droplet on superhydrophobic surfaces for aggregation and nucleation studies. Some models neglect Marangoni effect [4] but it can be included in the model by considering the non-uniformity of temperature. So, the heat equation can numerically be solved for the droplet domain in order to deduce the free surface tension gradient on the free surface. This last variable and the evaporation flux will be used as boundary conditions to solve the Stokes-equations inside the droplet domain. In particular, in a superhydrophobic surface the temperature gradient is totally different than in a hydrophilic one: this, obviously, induce a Maragoni effect given by a different surface tension gradient.

Reference

(1) “In Situ X-ray Scattering Studies of Protein Solution Droplets Drying on Micro- and Nano-patterned Super-hydrophobic PMMA Surfaces”, A. Accardo, F. Gentile, E. Di Fabrizio et Al., Langmuir 2010, 26(18), 15057–15064.

(2) Natural tri-to hexapeptides self-assemble in water to amyloid β-type fiber aggregates by unexpected α-helical intermediate structures. C. Hauser, R. Deng, A. Accardo et Al., PNAS,2011, 108 (4) 1361-1366.

(3) “Evaporation of a sessile droplet on a substrate”. H. Hua, R.Larson. Journal of Physical Chemestry. 2002, 106, 1334-1344.

(4) “Analysis of the Microfluid Flow in an Evaporating Sessile Droplet”, H.Hua, R. Larson. Langmuir 2005,21, 3963-3971

Figures used in the abstract

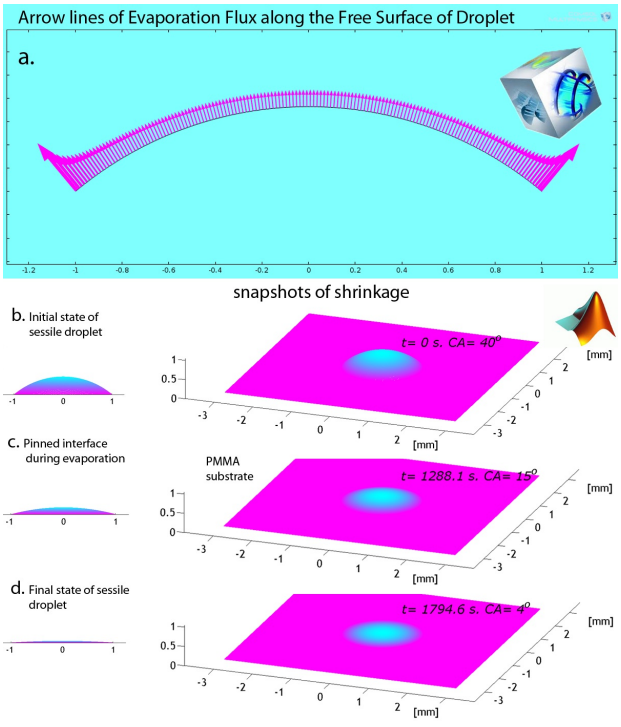

Figure 1