Dynamics of a Sessile Droplet Evaporation

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Introduction: Evaporation of sessile droplets is often associated to the so called "coffee ring" effect. The deposit shape depends on the flows nature inside the droplet and the prediction of the inner velocity fields can help to understand how colloids deposit on the substrate. Here a numerical simulation was made to obtain the evaporation flux profile along the free surface which plays a key role in the formation of amyloid β-fiber aggregates [1,2].

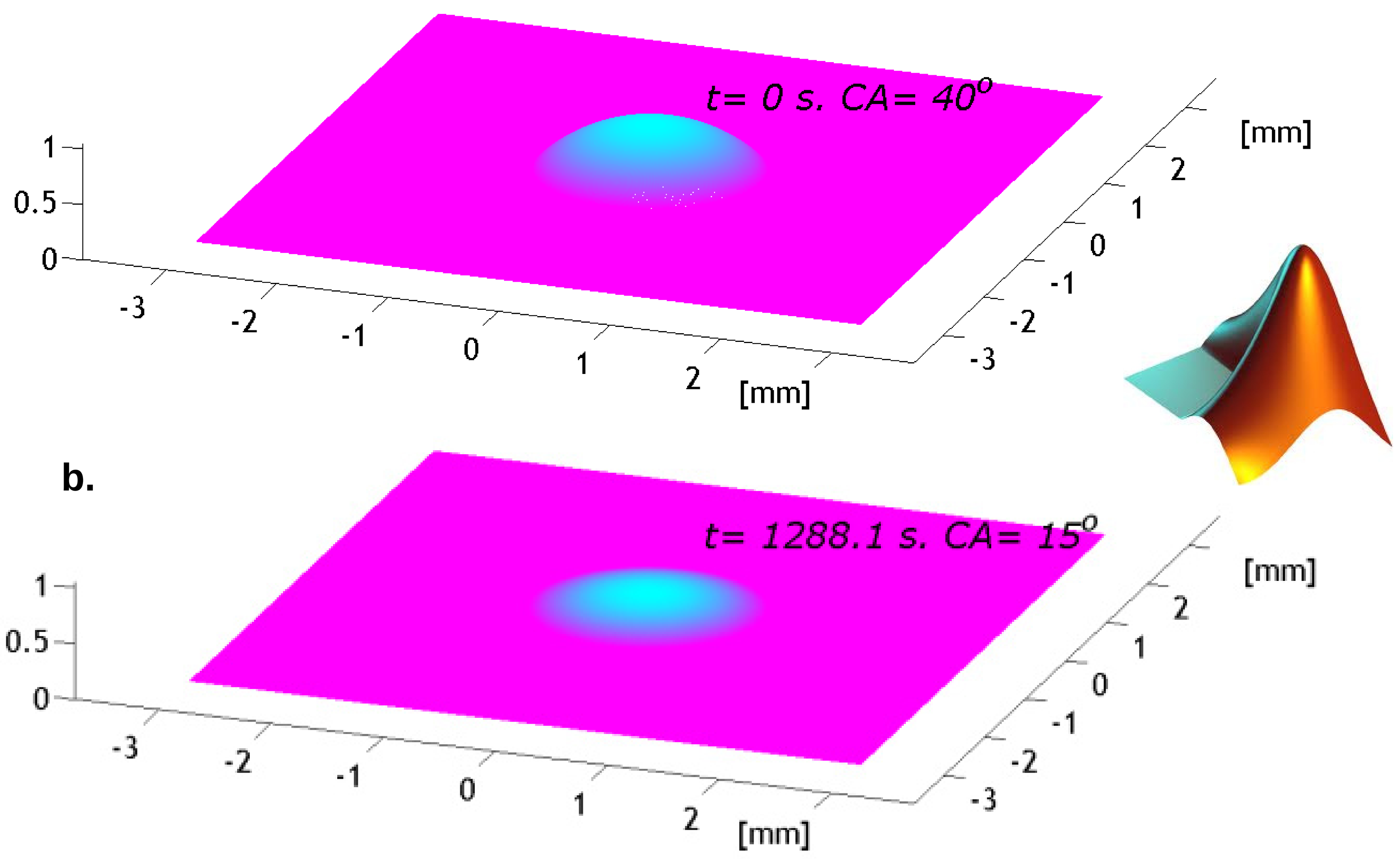


Figure 1. **(a)** Initial state of a 4uL sessile water droplet on a PMMA surface. Contact Angle (CA) is 40°. **(b)** Snapshot of the shrinking evolution obtained in MATLAB. A similar movie is obtained in Comsol with the moving mesh (Arbitrary Lagrangian-Eulerian Method)

Computational Methods: The system can be considered with an axisymmetric geometry.

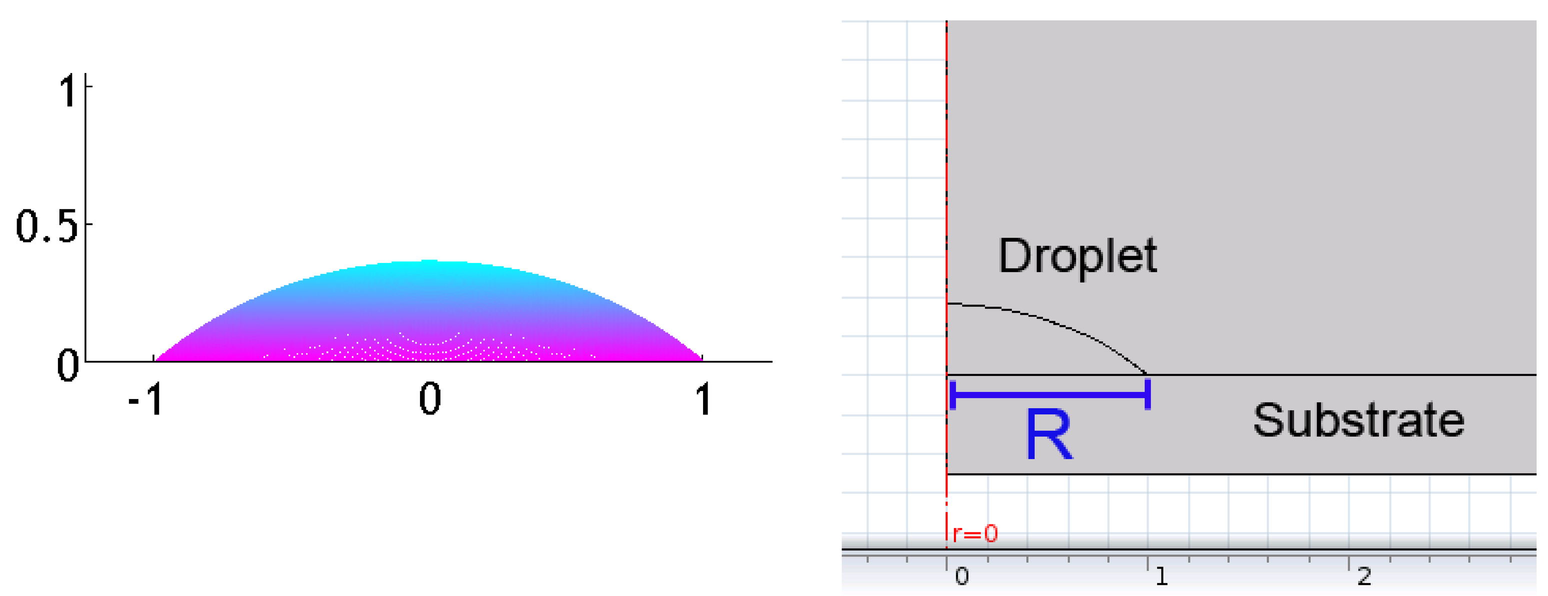


Figure 2. Spherical cup geometry. During evaporation, droplet remains pinned

Aqueous vapor concentration changes and settles rapidly respect to the time of evaporation and whenever the droplet shape changes. For this reason the evaporation was thought to be a quasi-steady-state process [3] and the "Second Fick Law" becomes:

$$\nabla \cdot \left(-D_i \nabla c_i\right) = 0$$

$$J_i = -D_i \nabla \cdot c_i$$

The limit of the domain over the free surface of the droplet is considered to be 20*R where the vapor concentration is the one of the surrounding environment.

Results: The numerical solution provides an evaporation profile that can explain the "coffee stain" effect.

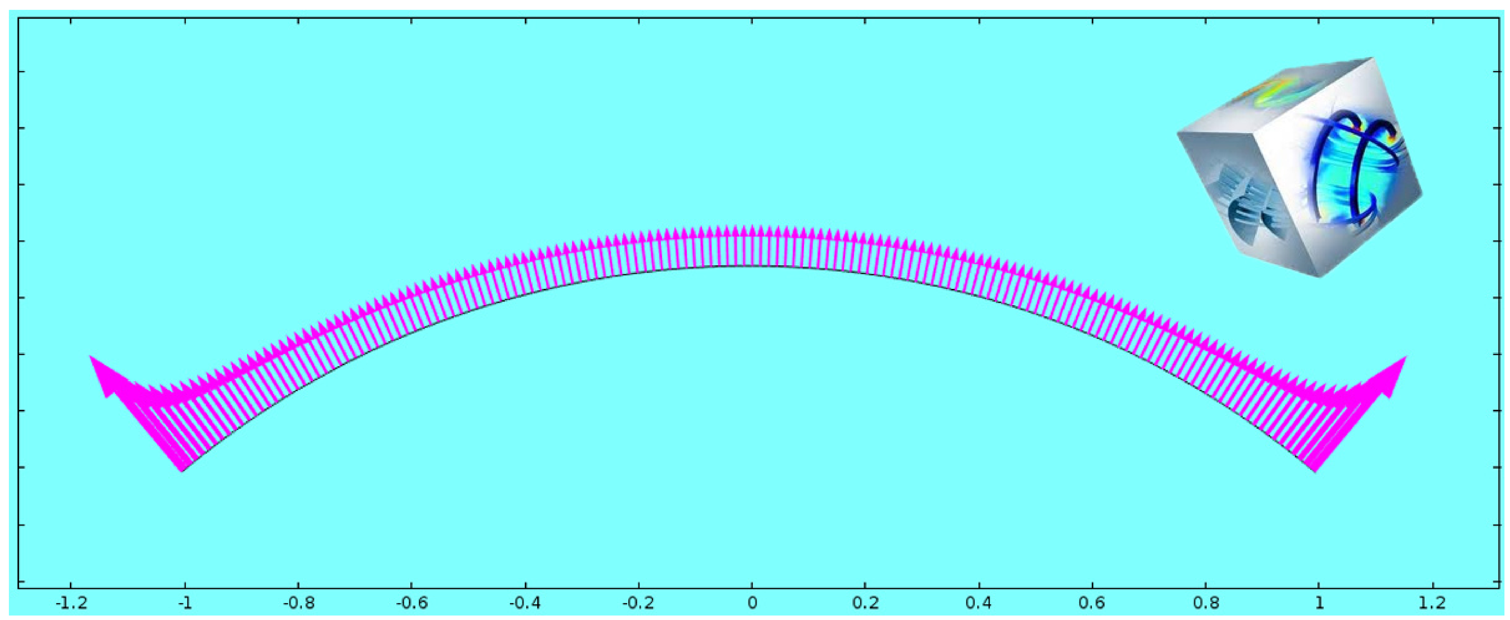
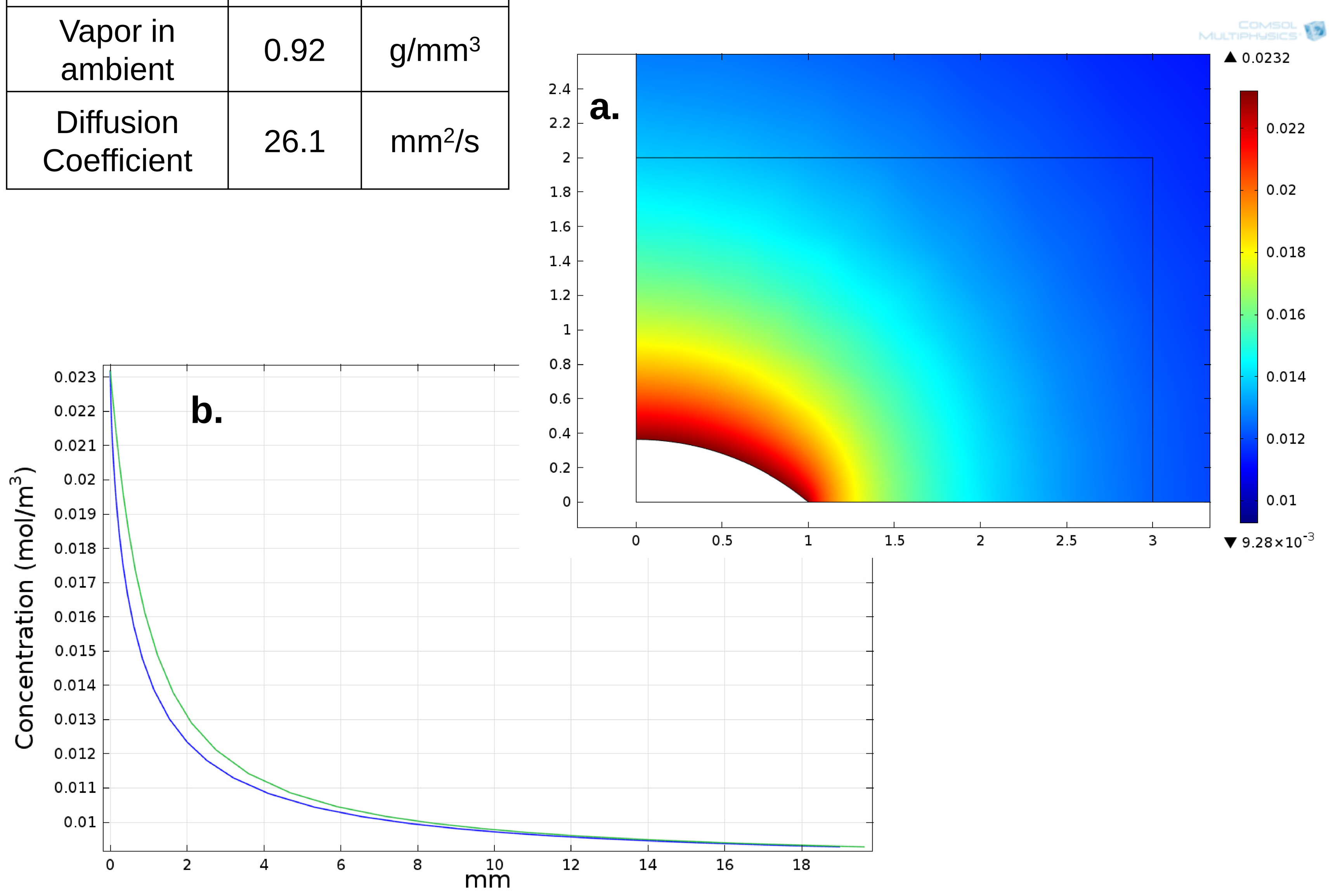


Figure 3. Arrow lines of evaporation flux along the Free Surface of Droplet. Evaporation Flux is greater at the edge of the droplet

Table of main parameters

	Value	Units
Free Surface Vapor	2.32e-9	g/mm^3
Vapor in ambient	0.92	g/mm^3
Diffusion Coefficient	26.1	mm^2/s

Figure 4 . (a) (b). Vapor concentration [mol/m^3]



Conclusions: Sessile Droplet evaporation depends on the wetting properties of the substrate. Here a low CA provides an evaporation flow greater at the edge and lower at the top surface of the droplet. On the other hand, when CA is greater than 90° the flow at the edge will result lower. Starting from previous studies [4], superhydrophobic surfaces will be used in further developments integrating both fluidodynamics and Marangoni effect inside the droplet.

References:

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2. **"Natural tri-to hexapeptides self-assemble in water to amyloid β-type fiber aggregates by unexpected α- helical intermediate structures.» C. Hauser 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.**
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