# Modeling capillary phenomena at a mesoscopic scale: from simple to complex fluids

**S. Merabia, J. Bonet Avalos and I. Pagonabarraga**
Universitat de Barcelona and Universitat Roviri i Virgili, Tarragona, Spain

Capillary phenomena are ubiquitous in nature and in industry as well [1]. From a theoretical point of view, the difficulty arises from the fact that these phenomena involve free boundaries. In this context, numerical simulations can help in the characterisation and understanding of the flow of drops or thin films. To this end different strategies have been pursued: either one solves the Navier Stokes equations with a structureless interface. This route fails in describing situations where singularities occur such as drop break up or the classical problem of the contact line dynamics [2]. To go beyond, molecular approaches *e.g.* molecular dynamics can be utilized [3, 4]. However, these methods are limited to small time (10 ns) and length scales (10 nm), thus making the hydrodynamic regime hard to reach.

In this presentation, we will introduce a mesoscopic model for the dynamics of interfaces, somewhere in between molecular dynamics and continuum mechanics. The fluid is represented as a set of effective particles interacting through soft forces allowing to gain orders of magnitude in the time scales reached with respect to molecular dynamics [5]. We will show how to account for the presence of a solid interface whose wetting properties can be tuned from hydrophilic to superhydrophobic. The performance of the model will be assessed by studying two classical capillary phenomena: the spreading of a drop on a hydrophilic substrate and the dewetting of a liquid thin film on a partially wetting solid. In both cases, very good agreement is found between the results of the simulations and the theoretical predictions [5].

We will study two applications of the proposed model: first we will concentrate on the dynamics of drops laying on a partially wetting substrate and which are deformed by an external force. For small forces (capillary numbers), we found that the drop keeps its ovale shape. If the force is increased, a cone appears at the rear of the drop whose aperture angle is a decreasing function of the velocity. On increasing further the velocity of the drop, no stationary state is reached and the drop emits small droplets as in the Rayleigh-Plateau instability. All these features have been also observed in recent experiments of drops sliding down an inclined plane [6]. Interestingly, both in the experiments [7] and in the simulations, the transition between a steady state shape and the pearling instability occurs for a non vanishing value of the receding contact angle contrary to an old belief. Note finally that these situations are fully relevant in coating processes.

The second application will involve the dewetting of polymer blends thin films. If the dewetting of simple fluids is now well characterised experimentally and interpreted theoretically, binary fluids can reveal novel dewetting scenarios yet not understood [8]. Little less is known regarding polymer blends. Note that most of the thin films used in industry are made of more than one component, it is thus relevant to adress such situations. In this presentation, we will show how to extend the proposed mesoscopic model to deal with complex fluids such as binary fluids and polymer blends. We will study the kinetics of dewetting of a polymer blend thin film as a function of the viscosities of the two components of the blend. The results of the simulations will be interpreted with a simple model [9]. Finally if time permits, we will talk about diblock copolymer thin films and study the interplay of mesophase formation and dewetting in these systems.

As a conclusion, we have introduced a mesoscopic model for the dynamics of capillary phenomena.

We have studied the ablity of the proposed model to capture subbtle effects such as drop break up under the action of external forces. We have also shown the versatility of the model to deal with complex fluids such as binary mixtures or polymer blends. We hope the work on binary mixtures and polymer blends will stimulate experiments in this direction.

**References :**

[1] De Gennes P. G., Brochard F. and Quéré D., *Capillary and wetting phenomena: drops, bubbles, pearls, waves* (Springer, New York, 2003)
[2] Eggers J., *Rev. Mod. Phys*. **69**, 865 (1997)
[3] Milchev A., Milchev A., Binder K., *Comput. Phys. Commun.,* **146** 38 (2002)
[4] Koplik J. and Banavar J. R., *Phys. Rev. Lett.,* **84** 19 (2000)
[5] Merabia S. and Pagonabarraga I., *Eur. Phys. J. E.*, **20** (2) 209 (2006)
[6] Podgorski T., Flesselles J.-M. and Limat L., *Phys. Rev. Lett.* **87** 036102 (2001)
[7] Le Grand N., Daerr A. and Limat L., *J. Fluid. Mech.* **541** 293 (2005)
[8] Yerushalmi-Rozen R., Kerle T. and Klein J., *Science* **285** (5431) 1254 (1999)
[9] Brochard F., di meglio J.M. and Quéré D., C. R. Acad. Sci. (Paris) **304**, 553 (1987)