Simulations of capillary systems

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Abstract: *The capillarity can be found in many systems. Here, we target two problems about (i) the occlusion of small airways in the lung and (ii) the applicability of capillarity theory to nanometric systems. We studied these problems by Monte Carlo and molecular dynamics simulations, respectively. In the study (ii) we focus on capillary bridge, which is a meniscus formed between two planar surfaces. In both studies the capillary theory provide good predictions to the results obtained from simulations. This study shows that capillary theory can be applied to both mesoscopic and nanoscopic systems.*

Key-Words*: capillary bridges, droplets, molecular dynamics, Monte Carlo*

Introduction: The capillarity theory (CT) uses continuum description to represent macroscopic interfaces formed between two immiscible liquids or between a liquid and a vapor [1]. The CT has several applications to macroscopic, mesoscopic and some nanoscopic systems, ranging from diagnosis of airways condition in the lung to wetting. In the lung, capillary bridges may form in the small airways blocking airflow due to abnormal mechanical instabilities [2]. The rupture (formation) of capillary bridges during inhalation (exhalation) are the major cause of the crackling adventitious lung sound, which can be heard using a simple stethoscope [3,4]. These capillary bridges have been studied in microfluidic devices to mimic the lung conditions [5,6]. The capillary bridges at the nanoscale are essential in many applications such as ink transfer in the dip-pen nanolithography [7], and imaging in atomic force microscopy [8]. This has motivated the understanding of the applicability of CT at this scale, where molecular details may become relevant, by computer simulations [9].

Experimental: Here, we conducted two studies in which the CT and numerical simulations were used to comprehend the processes of occlusion of small airways in the lung [4], and to test the applicability of capillarity concepts to nanoscopic systems [9]. In the first study, we focus on the blocking of airflow of small airways due to the formation of capillary bridges. To understand this phenomenon, we study axisymmetric capillary bridges (AS bridges) attached between two parallel walls by performing Monte Carlo simulation of a lattice gas model. In the second study, we perform atomistic Molecular Dynamics (MD) simulations of water droplets and capillary bridges of different symmetry in contact with various hydroxilated silica walls, which are modified to cover a wide range of hydrophobicity/hydrophilicity. In both studies calculate the main properties of the system such as profiles, contact angle, capillary adhesion force and Laplace pressure.

Results and discussion: In the first study, the simulation results are in agreement with the CT predictions, and we observed a difference in free energy prior and after the bridge formation, indicating the cause of the crackling adventitious lung sound. We also observed an hysteresis in the free energy with two gaps, and it is in agreement with CT. In the second study, we have shown that CT provides satisfactory predictions of droplets and bridges shapes formed by volumes in the order of 100 nm^3. We observed that the water contact angle is independent of the droplet/bridge geometries and it depends only on the hydrophobicity/hydrophilicity of the walls. The capillary adhesion force and the Laplace pressure were in accord with CT. We noticed that the Laplace pressure can be very large ~250 atm for hydrophobic surfaces, or very low ~150atm for hydrophilic surfaces. These values of pressures can be predicted by Young-Laplace equation. The water surface tension calculated by using CT is close to the values found in the literature [10].

Conclusion: From the first study we observed that the release of free energy due to the liquid bridge formation is related to the generation of crackling sounds. We notice that the free energy difference is proportional to the contact angle, and hence it may be related to properties of coating fluids in small airways. From the second study, we have found good agreement between MD simulation and CT for volumes in order of 100 nm^3. The

validation of CT at such small scales is notable since CT is a macroscopic theory based on continuum surfaces, and this approach is expected to fail at nanoscales.

References and acknowledgements:

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