

Summary

The dynamics wetting of fiber is of crucial importance in the fields, such as composites, optical fiber or textile industries. It is therefore valuable to acquire a clear understanding of the fundamental physical mechanisms which govern this phenomenon. In the case of partial wetting, it is assumed that the loss of energy due to the change in shape of the liquid-fluid interface (surface tension) is balanced by two channels of dissipation. One is associated with the viscosity of the liquid (hydrodynamics), whereas the other is due to the friction between the liquid and the solid (molecular-kinetic theory). Translated into equations, this original approach leads to the conclusion that the friction regime should precede the hydrodynamic one for a low viscosity liquid. The crossover time between the two regimes is calculated and shown to be material dependent. To validate these theoretical predictions, both experiments and large scale molecular dynamics simulations of the spontaneous spreading of a liquid along a fiber are run. The experiments consist in capturing images of meniscus formation around the fiber via a high speed camera. For each image, the liquid-air profile is extracted and fitted to a solution of the Laplace equation yielding the contact angle and the height of the meniscus as a function of the time. For low viscosity liquid it is found that the measured dynamic contact angle follows the friction regime, whereas for higher viscosity liquid the viscous regime is recovered as presented theoretically. The same kind of procedure is followed to study the wetting of a nanofiber by molecular dynamics. The properties of the liquid are first assessed (viscosity, shape of the molecule, molecular volume). Because of the very low viscosity of the model liquid, it is expected that the friction between the liquid and the solid is the dominant channel. Indeed, the data from the simulation validates this assumption. Moreover, according to the results of the simulation, it is also confirmed that for a given equilibrium contact angle, a maximum of speed wetting occurs. Actually, a low (or high) equilibrium contact angle involves both a strong (or weak) driving force and adhesion of the liquid molecules to the solid atoms. These opposite effects do not simply cancel out and therefore lead to the existence of a maximum rate at which a liquid can wet a solid.

To examine in detail this last statement, the forced wetting of fiber is studied by molecular dynamics. The fiber, at a constant velocity, goes through the meniscus of a liquid which is consequently elongated. Stationary receding and advancing contact angles are then measured as a function of the fiber velocity. It is found that the contact angle dependence on the fiber velocity follows the molecular-kinetic theory, thereby confirming the existence of a maximum. Moreover, a comparison between the values of the microscopic parameters obtained via the adjustment of the theory and a direct measurement of these parameters permits us to check the validity of the chosen theory as well as the reliability of the simulation tool.

Finally in order to study the wetting of fibrous materials like fabrics, an effective system is studied via molecular dynamics. It is shown that the measurements of capillary imbibition and droplet spreading are well modelled by a set of equations taking into account the conservation of the volume of the liquid, the influence of a dynamic contact angle inside the pore and the spreading on top of the surface. This single pore geometry is extended theoretically to the case of multiple non-interconnected pores. The time required to absorb the droplet completely is then calculated.