Test-case number 6: Two-dimensional droplet pining on an inclined wall (PC)

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1 Practical significance and interest of the test-case

In many experimental situations, see *e.g.* (Dussan, 1976) or (Carey, 1992), the actual value of the static contact angle is a consequence of the past motion of the contact line, before its pining: this phenomenon is called the hysteresis of the contact angle, for the value is usually higher for a (previously) advancing contact line than for a (previously) receding contact line. The amplitude of the hysteresis, that is the difference between the advancing and the receding contact angles, is mainly due to effects that arise at scales smaller than the micrometer, especially effects of wall roughness and effects of non-homogeneous chemical composition of the solid surface or contamination. These small-scale physicochemical phenomena only affect the macroscopic scales through the apparent contact angle and its hysteresis. Taking into account the effects of the unresolved physics with a macroscopic model is a classical approach in Direct Numerical Simulation techniques.

This test-case is only qualitative and is primarily dedicated to test the ability of a numerical method to simulate contact line effects and the contact line hysteresis in particular. The original test-case can be found in (Duquennoy, 2000) and (Duquennoy *et al.* , 2000). The main goal of the test-case is to qualify and illustrate the ability of a numerical method to cope with the contact line hysteresis and to take into account the values of the advancing and receding contact angles.

The main idea of the test-case is to check the onset of sliding of a droplet on an inclined surface. In a two-dimensional simulation, balance between gravity (droplet weight) and surface tension (contact angles) effects results in a limiting value for the angle of inclination of the surface on which the droplet is standing. This simplicity is apparent, because the onset conditions are usually not reached on both contacts for the same value of the inclination (Feuillebois, 2000). However, making the assumption of a simultaneous onset on both contacts provides a reasonable estimate (Duquennoy, 2000). Moreover, the double procedure proposed to determine the limiting angle, and explained in the last section of this test-case, gives an estimate of the validity of this assumption. This test-case is therefore *not* an accurate validation of the implementation of the contact line effects, but is nevertheless easy to perform and can provide a decent qualitative qualification.

2 Description of the model for the contact angle hysteresis and definition of the test-case

The simplest way to describe a macroscopic contact angle which undergoes a hysteretical behavior is

$$\begin{cases} \theta_{app} = \theta_A & \text{if } V > 0 \\ V = 0 & \text{while } \theta_R < \theta_{app} < \theta_A \\ \theta_{app} = \theta_R & \text{if } V < 0 \end{cases} \tag{1}$$

where θ_{app} is the macroscopic contact angle, θ_A and θ_R are the advancing and receding contact angles respectively and V is the speed of displacement of the contact line.

The test-case consists in computing the conditions for which of a two-dimensional droplet sticks or slides on an inclined wall. Let us denote α the angle between the horizontal direction and the inclined wall. For a given hysteresis, that is for a given set (θ_A, θ_R), the inclination has a limit value α_{lim} so that the droplet may stay at rest on the wall. A balance between gravity and surface tension forces characterizes this equilibrium. Since we consider the two-dimensional case, the marginal equilibrium is approximately given by

$$sin\left(\alpha_{lim}^{theory}\right) = -\frac{\sigma}{\left(\rho_L - \rho_G\right) g V_{droplet}} \left(cos\left(\theta_A\right) - cos\left(\theta_R\right)\right), \tag{2}$$

where $V_{droplet}$ is the volume (surface) of the droplet, ρ_L and ρ_G are respectively the density of the droplet liquid and the density of the surrounding gas, σ is the surface tension between the gas and the liquid and g is the gravity intensity. The physical fluid model is reduced to the Navier-Stokes equations in both phases, with a constant surface tension at the interface. The simplest choice for the other physical properties is constant densities ρ_L and ρ_G, constant dynamic viscosities μ_L and μ_G. Another basic assumption states that no phase-change takes place at the interface. Since the solution does not depend on a possible compressibility of one or both of the phases, the test-case can be conducted in both cases (compressible / incompressible), depending on specific features of the numerical method to be tested. A further simplification is even possible (if needed) by neglecting the gas phase (*e.g.* $\rho_G = 0$ and $\mu_G = 0$). A simple initial shape is a half circle. Both fluids may also be initialized at rest.

The test may be conducted with any convenient set of physical parameters, because equation (2) provides a good estimate in most situations. However, a typical set is suggested, which approximately corresponds to the values for air and water at room temperature: $\rho_L = 958$ kg.m^{-3}, $\mu_L = 282\ 10^{-5}$ Pa.s, $\rho_G = 0.59$ kg.m^{-3}, $\mu_G = 12.3\ 10^{-5}$ Pa.s, $\sigma = 59\ 10^{-3}$ N.m^{-1}, $g = 9.81$ m.s^{-2}. In addition to those values, the hysteresis defined in (Duquennoy, 2000) is: $\theta_A \approx 85.94^\circ$ (1.5 rad), $\theta_R \approx 22.92^\circ$ (0.4 rad). The last parameter is the radius of the initial half circle d_e and therefore the value of the surface $V_{droplet}$. A value of $d_e = 2$ mm ($V_{droplet} \approx 6.28$ mm^2) is suggested. For this set of values, an approximate solution for the limit angle of equilibrium is $\alpha_{lim}^{theory} \approx 58.2^\circ$ (≈ 1.01 rad).

3 Test procedure

The aim of the test is to find an estimate of the limit angle α_{limit}. The test has to be conducted in two steps:

- In a first step of the procedure, the equilibrium shape of a droplet is found for an inclination α smaller than θ_R. A transient step-by-step increase of this angle allows to determine a lower bound for the limit angle α_{lim}: α_{lim}^{lower}. For all the values of the test angle α lower than α_{lim}^{lower}, the droplet is able to reach an equilibrium state, the shape of the interface depending on the value of α. Stepping should be performed carefully, especially in the case of low viscosities and when approaching the limit value α_{lim}^{lower}. The result of a rough stepping is to under-estimate the value of α_{lim}^{lower}. Additional attention should be paid to the mesh size used for the computation: When the mesh is too coarse, the result is usually erratic for a slight change in the value of the angle α.
- In the second step of the procedure, the upper limit for α_{lim} is searched: α_{lim}^{upper}. Computations are performed with values of α decreasing down to α_{lim}^{upper}. This limit is more difficult to determine than α_{lim}^{lower}, because it is not a succession of quasi-steady states. However, its allows to get an estimate of the uncertainty that subsists on the determination of α_{lim}.

4 Comparison criteria

The reduced difference ϵ_1 between the numerically estimated limit for the angle α_{lim}^{lower} and its theoretical value α_{lim}^{theory} given by equation (2), is a good measure of the quality of the numerical implementation of the hysteresis:

$$\epsilon_1 = \frac{\left|\alpha_{limit}^{lower} - \alpha_{limit}^{theory}\right|}{(\theta_A - \theta_R)}. \tag{3}$$

The reduced difference ϵ_2 between the numerically estimated upper and lower limits of the angle α_{lim} is a good measure of the quality of the assumption of a simultaneous onset of both contact lines:

$$\epsilon_2 = \frac{\alpha_{limit}^{upper} - \alpha_{limit}^{lower}}{(\theta_A - \theta_R)}. \tag{4}$$

According to (Duquennoy, 2000), $\epsilon_1 = 1\%$ and $\epsilon_2 = 5\%$ is a very good result.

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