BDGS: A Python code for solving binary drop shape

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Abstract

When two immiscible droplets come in contact, they form an interface and take a global shape that can range from a dumbbell shape to encapsulated shape. Here we present a Python-based solver of binary drop shape based on the work of Assovskii and Rashkovskii 2002 [1]. We have extended their work to droplets with variable volumes.

Keywords: droplets, coalesce, growth, shape

Theory and Methodology

Binary drop formation

When two immiscible droplets (1 and 2) come in contact, they create a nonequilibrium binary drop (Fig. 1), with a common interface (3). The drop is nonequilibrium since it would have unbalanced forces at the interface. As the forces balance, the drop evolves into an equilibrium shape (Fig. 2).

The following describe the binary drop geometry: (R_1,h_1), (R_2,h_2) and (R_3,h_3) are radius and minor cap height of the first fluid, second fluid and the interface respectively. R_b is the base radius of interface. Each of these are dimensionless, being normalized with effective drop radius R_0. The following geometric identities apply:

$$R_i = \frac{h_i^2 + R_b^2}{2h_i}, \quad i = 1, 2, 3. \tag{1}$$

If α is ratio of volume of second fluid to first fluid, β_2 is ratio of surface tension of second fluid to first fluid and β_3 is ratio of interface tension to surface tension of first fluid, then the equations of volume of first fluid and second fluid and force balance at interface give [1]:

$$R_1^3 - \frac{1}{8}h_1(h_1^2 + 3R_b^2) - \frac{1}{8}h_3(h_3^2 + 3R_b^2) = 1, \tag{2}$$

$$\frac{1}{8}h_2(h_2^2 + 3R_b^2) + \frac{1}{8}h_3(h_3^2 + 3R_b^2) = \alpha, and \tag{3}$$

$$\frac{\beta_2}{R_2} - \frac{1}{R_1} = \frac{\beta_3}{R_3}. \tag{4}$$

Nonequilibrium binary drop For a give parameter set (α, β_2,β_3), we can obtain nonequilibrium shapes of the drop by solving equations (eq. 1-4) for (R_1,R_2,R_3) for certain forced R_b. Generally there are 5 solutions, but 4 of them have high curvatures at the triple point (A in Fig. 2). The initial guess for the variables can be chosen such that experimentally/physiologically relevant shape is obtained. With this shape as the initial configuration, we can obtain the equilibrium drop shape as follows.

Equilibrium binary drop For a give parameter set (α, β_2,β_3), we can obtain equilibrium shape of the drop by solving equations (eq. 1-4) along with eq. 6 for (R_b,R_1,R_2,R_3) with the nonequilibrium shape as initialization.

Binary drop growth

In the above, it was assumed that the volume of the drops are fixed; hence R_0 and α were constants. Below, we describe an approach to solve for the trajectory of evolution of growing binary drop from an initial equilibrium binary drop through a small extension to the process above.

Evolution of drop shape The trajectory of evolution of drop shape from the nonequilibrium binary drop to the equilibrium drop can be obtained through quasi-static reduction of unbalanced tension at the triple point. Here,

$$R_0 = 1, \quad W_1 = \frac{4\pi}{3}, \quad W_2 = \alpha W_1. \tag{5}$$

Growing binary drop Similarly, once we obtain initial equilibrium shape of the drop as described above, we can obtain the next shape after time dt with the updated α and R_0 as follows:

$$W_1 {+}{=}\, g_1 dt, \quad W_2 {+}{=}\, g_2 dt, \quad \alpha = W_2/W_1, \quad R_0 = \sqrt[3]{\frac{3W_1}{4\pi}}. \tag{6}$$

Results

The following are results of the simulations:

1. `https://github.com/modelsbox/BDGS/blob/main/relaxation/fig/drop.gif` demonstrates an example binary drop formation, and

2. `https://github.com/modelsbox/BDGS/blob/main/growth/fig/drop.gif` demonstrates an example binary drop growth.

References

[1] Assovskii, I. G., and S. A. Rashkovskii. 2002. "Relaxation of Drops of a Mixture of Two Immiscible Liquids to Equilibrium Shapes." Doklady Physical Chemistry 385(1–3): 149–53.

Figures

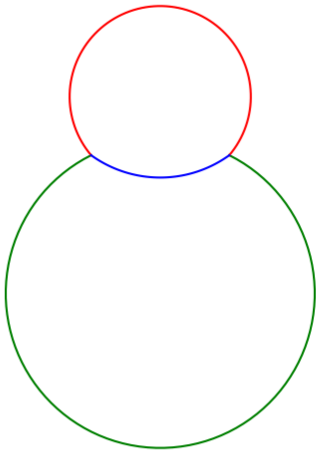

Figure 1: **The nonequilibrium binary drop.** Two droplets forming an interface upon contact.

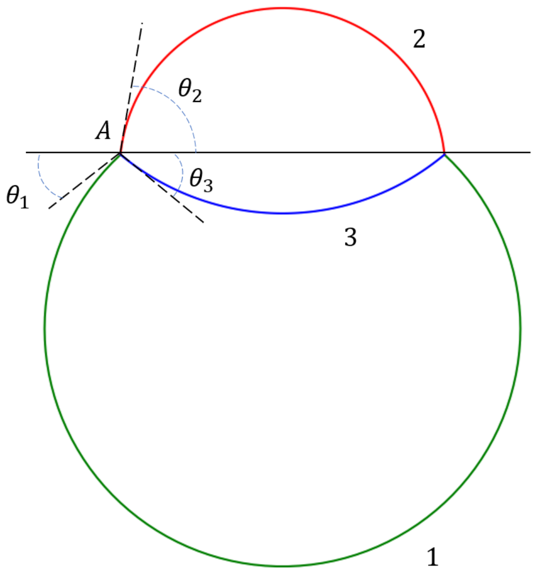

Figure 2: **The equilibrium binary drop.** Geometric features labeled.