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Generalized Young Equation for Cylindrical Droplets within a Homogeneous and Smooth Regular Triangular Prism Filled with Gas in Three Convex Corners

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Abstract

Based on the approaches of Gibbs's dividing surface and Rusanov's dividing line, the wetting behaviors of cylindrical droplets that at equilibrium are sitting inside a homogeneous and smooth regular triangular prism filled with gas in three convex corners are studied. For the three-phase system, which is composed of solid, liquid and gas phases, a generalized Young equation for cylindrical drops in a homogeneous and smooth regular triangular prism imbued with gas within three apex corners has been successfully derived including the effects of the line tension.

Keywords: generalized Young equation; cylindrical droplet; line tension; regular triangular prism; convex corner

1. Introduction

Wetting is one of the most important behaviors of solid surfaces and plays a critical role in daily lives and industrial applications, such as self-cleaning windows and antifouling surfaces (Li & Amirfazli, 2005; Ebert & Bhushan, 2012; Li et al., 2010), nanofluids (Balakin et al., 2015), carbon nanotubes (Ghadyani & Öchsne, 2015), biomaterials (Rupp et al., 2014), and evaporation (Li et al., 2014). The Wettability of a solid by a liquid may be represented by using the contact angle between the gas-liquid and solid-liquid interfaces. For a chemically homogeneous and smooth flat surface, the contact angle is given by Young's equation (Young, 1805)

$$\cos\theta_Y = \frac{\sigma_{SG} - \sigma_{SL}}{\sigma_{LG}} \tag{1}$$

where σ_{SG}, σ_{SL} and σ_{LG} are the interfacial tensions of solid-gas, solid-liquid, and liquid-gas, separately.

The wetting of liquids on a rough surface in general is investigated by one of the following two models: in the Cassie model (Cassie & Baxter, 1944), the drop remains suspended beyond the asperities of the solid surface, and in the Wenzel model (Wenzel, 1936), the drop penetrates into the asperities of the corresponding surface. The aforementioned Young equation, the Cassie and Wenzel models build the theoretical foundation of wetting studies.

In the past two decades, scholars have shown great interest in the wetting properties of solid surfaces and carried out a great deal of related studies (Patankar, 2003; Dumitrascu & Borcia, 2006; Boinovich & Emelyanenko, 2011; Zhu et al., 2013; Yano & Nishino, 2015). However, until now, there is still not the generalized Young's equation for cylindrical droplets inside a homogeneous and smooth regular triangular prism filled with gas in three apex corners. Therefore, the purpose of this paper is to thermodynamically derive a generalized Young equation for contact angles of cylindrical droplets within a homogeneous and smooth regular triangular prism, which is imbued with gas in three corners.

2. Calculating the Systematic Free Energy

Considering a cylindrical drop (phase L) with single component in contact with its gas (phase G), placed within a homogeneous and smooth regular triangular prism (phase S) with both gas in three corners and sides of length L, as illustrated in Figure 1.

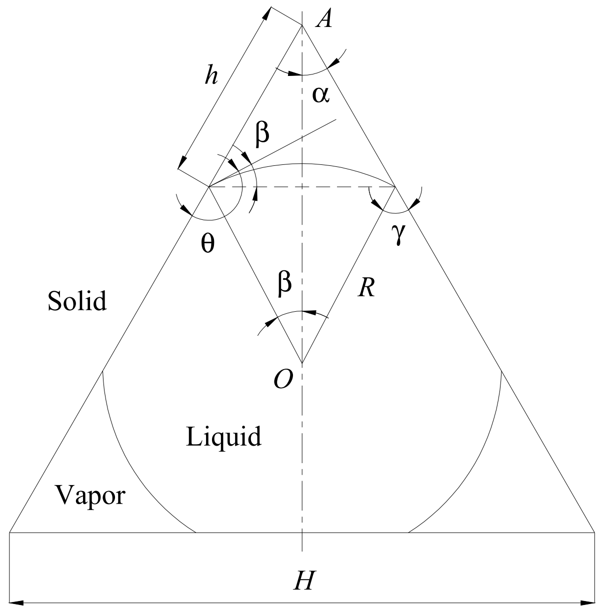

Figure 1. A cylindrical droplet in a homogeneous and smooth regular triangular prism filled with gas within three corners

Using the method of Gibbs's dividing surface, the system shown in figure 1 contains six phases: liquid phase, gas phase, solid-liquid interface, solid-gas interface, liquid-gas interface, and the three-phase line. And then, the total Helmholtz free energy F can be expressed as

$$F = F_L + F_G + F_{SL} + F_{SG} + F_{LG} + F_{SLG} \tag{2}$$

where F_L, F_G, F_{SL}, F_{SG}, F_{LG} and F_{SLG} being the Helmholtz free energies of the above six phases, respectively, the subscripts being the quantities relate to the homologous phases, interfaces along with the triple phase line (for example, the subscripts *G* and *SL* mark the gas phase and solid-liquid, respectively), separately.

The Helmholtz free energies of various phases are written as (Rowlinson & Widom, 1982)

$$F_L = -p_L V_L + \mu_L N_L \tag{3}$$

$$F_G = -p_G V_G + \mu_G N_G \tag{4}$$

$$F_{SL} = \sigma_{SL} A_{SL} + \mu_{SL} N_{SL} \tag{5}$$

$$F_{SG} = \sigma_{SG} A_{SG} + \mu_{SG} N_{SG} \tag{6}$$

$$F_{LG} = \sigma_{LG} A_{LG} + \mu_{LG} N_{LG} \tag{7}$$

$$F_{SLG} = kL_{SLG} + \mu_{SLG} N_{SLG} \tag{8}$$

where p is the pressure, V is the volume, μ is the chemical potential, N is the mole number of molecule, A is the interfacial area, σ is the interfacial tension, k is the line tension, and L is the length of the triple phase line.

Ignoring the effects of both the gravity and the other forces or fields, therefore, the balanced shape of the cylindrical droplet in Figure 1 is that of combining a hexagonal prism and three cylindrical fractions, each similar to a cylindrical cap.

The liquid volume V_L is

$$V_L = \frac{1}{2} H^2 L \cos\alpha - 3R^2 L \sin^2\beta \frac{\cos\alpha}{\sin\alpha} + 3R^2 L\left(\beta - \sin\beta\cos\beta\right) \tag{9}$$

here H, L and α are the side length, height and semiapex angle of the regular triangular prism, separately, R is the radius of the cylindrical droplet, and β is the apparent contact angle.

The total systematic volume V_t is

$$V_t = V_L + V_G \tag{10}$$

The liquid-gas interfacial area A_{LG} is

$$A_{LG} = 6RL\beta \tag{11}$$

The solid-liquid interfacial area A_{SL} is

$$A_{SL} = 3HL - 6RL\frac{\sin\beta}{\sin\alpha} \tag{12}$$

The sum A_t of the solid-liquid and solid-gas interfacial areas is

$$A_t = A_{SL} + A_{SG} \tag{13}$$

The length of the three-phase line is

$$L_{SLG} = 6L \tag{14}$$

Using Eqs. (9-14) and Eqs. (3-8) before, we obtain

$$F_L = -p_L \cdot \left[\frac{1}{2}H^2 L\cos\alpha - 3R^2 L\sin^2\beta\frac{\cos\alpha}{\sin\alpha} + 3R^2 L\left(\beta - \sin\beta\cos\beta\right)\right] + \mu_L N_L \tag{15}$$

$$F_G = -p_G \cdot \left\{V_t - \left[\frac{1}{2}H^2 L\cos\alpha - 3R^2 L\sin^2\beta\frac{\cos\alpha}{\sin\alpha} + 3R^2 L\left(\beta - \sin\beta\cos\beta\right)\right]\right\} + \mu_G N_G \tag{16}$$

$$F_{SL} = \sigma_{SL} \cdot \left(3HL - 6RL\frac{\sin\beta}{\sin\alpha}\right) + \mu_{SL} N_{SL} \tag{17}$$

$$F_{SG} = \sigma_{SG} \cdot \left(A_t - 3HL + 6RL\frac{\sin\beta}{\sin\alpha}\right) + \mu_{SG} N_{SG} \tag{18}$$

$$F_{LG} = \sigma_{LG} \cdot 6RL\beta + \mu_{LG} N_{LG} \tag{19}$$

$$F_{SLG} = 6L \cdot k + \mu_{SLG} N_{SLG} \tag{20}$$

Now substituting the above Eqs. (15-20) into Equation (2), we have

$$\begin{aligned} F = &-\left(p_L - p_G\right)\cdot\left[\frac{1}{2}H^2 L\cos\alpha - 3R^2 L\sin^2\beta\frac{\cos\alpha}{\sin\alpha} + 3R^2 L\left(\beta - \sin\beta\cos\beta\right)\right] \\ &- p_G \cdot V_t + \sigma_{LG}\cdot 6RL\beta + \left(\sigma_{SL} - \sigma_{SG}\right)\cdot\left(3HL - 6RL\frac{\sin\beta}{\sin\alpha}\right) + \sigma_{SG}\cdot A_t + 6L\cdot k \\ &+ \mu_L N_L + \mu_G N_G + \mu_{LG} N_{LG} + \mu_{SL} N_{SL} + \mu_{SG} N_{SG} + \mu_{SLG} N_{SLG} \end{aligned} \tag{21}$$

3. Derivation of a Generalized Young's Equation

The grand thermodynamic potential Ω of the above three-phase system can be written as

$$\Omega = F - \sum_i \mu_i N_i \tag{22}$$

where the sign i stands for the phase number of the investigated system.

Putting Equation (21) into Equation (22) leads to

$$\begin{aligned} \Omega = &-\left(p_L - p_G\right)\cdot\left[\frac{1}{2}H^2 L\cos\alpha - 3R^2 L\sin^2\beta\frac{\cos\alpha}{\sin\alpha} + 3R^2 L\left(\beta - \sin\beta\cos\beta\right)\right] \\ &- p_G \cdot V_t + \sigma_{LG}\cdot 6RL\beta + \left(\sigma_{SL} - \sigma_{SG}\right)\cdot\left(3HL - 6RL\frac{\sin\beta}{\sin\alpha}\right) + \sigma_{SG}\cdot A_t + 6L\cdot k \end{aligned} \tag{23}$$

By minimizing the grand potential Ω with respect to the radius R, we obtain

$$\left[\frac{d\Omega}{dR}\right] = 0 \tag{24}$$

Due to the interfacial tensions σ_{SL} and σ_{SG} independent of dividing surfaces, there are the following constraints (Rusanov et al., 2004)

$$\left[\frac{d\sigma_{SL}}{dR}\right] = 0,\ \left[\frac{d\sigma_{SG}}{dR}\right] = 0 \tag{25}$$

Substituting Equation (23) into Equation (24) and using Equation (25), we can write

$$
\begin{aligned}
&-\left(p_L - p_G\right)\cdot\left[\frac{dV_L}{dR}\right]+\left[\frac{d\sigma_{LG}}{dR}\right]\cdot A_{LG}+\sigma_{LG}\cdot\left[\frac{dA_{LG}}{dR}\right]\\
&+\left(\sigma_{SL}-\sigma_{SG}\right)\cdot\left[\frac{dA_{SL}}{dR}\right]+\left[\frac{dk}{dR}\right]\cdot L_{SLG}+k\cdot\left[\frac{dL_{SLG}}{dR}\right]=0
\end{aligned} \tag{26}
$$

The following expressions can be obtained from Figure 1

$$R\sin\beta = h\sin\alpha \tag{27}$$

$$h\cos\alpha + R\cos\beta = \overline{OA} = const \tag{28}$$

$$\begin{cases}\gamma = \alpha+\beta\\ \theta = \gamma + \dfrac{\pi}{2}\end{cases} \tag{29}$$

and

$$\frac{d\beta}{dR} = -\frac{\sin\left(\alpha+\beta\right)}{R\cos\left(\alpha+\beta\right)} \tag{30}$$

$$\frac{dh}{dR} = -\frac{1}{\cos\left(\alpha+\beta\right)} \tag{31}$$

According to Eqs. (9, 11, 12, 14, 30, 31), there have

$$\left[\frac{dV_L}{dR}\right] = 6RL\beta \tag{32}$$

$$\left[\frac{dA_{LG}}{dR}\right] = 6L\beta - 6L\cdot\frac{\sin\left(\alpha+\beta\right)}{\cos\left(\alpha+\beta\right)} \tag{33}$$

$$\left[\frac{dA_{SL}}{dR}\right] = \frac{6L}{\cos\left(\alpha+\beta\right)} \tag{34}$$

$$\left[\frac{dL_{SLG}}{dR}\right] = 0 \tag{35}$$

There is a general Laplace equation applicable to the cylindrical liquid drop in Figure 1 (Rowlinson & Widom, 1982)

$$p_L - p_G = \frac{\sigma_{LG}}{R} + \left[\frac{d\sigma_{LG}}{dR}\right] \tag{36}$$

Putting Eqs. (32-36) into Equation (26) yields

$$\sin\left(\alpha+\beta\right) = \frac{\sigma_{SL}-\sigma_{SG}}{\sigma_{LG}} + \frac{\cos\left(\alpha+\beta\right)}{\sigma_{LG}}\cdot\left[\frac{dk}{dR}\right] \tag{37}$$

Substituting Equation (29) into Equation (37) arrives at

$$\cos\theta = \frac{\sigma_{SG}-\sigma_{SL}}{\sigma_{LG}} - \frac{\sin\theta}{\sigma_{LG}}\left[\frac{dk}{dR}\right] \tag{38}$$

After comparing Equation (1) with Equation (38), we get

$$\cos\theta = \cos\theta_Y - \frac{\sin\theta}{\sigma_{LG}}\left[\frac{dk}{dR}\right] \tag{39}$$

Therefore, for cylindrical droplets sitting within a homogeneous and smooth regular triangular prism filled with gas in three corners, Equation (39) is the generalized Young's equation that can be applied to random interfaces dividing the liquid and gas phases.

4. Conclusion

In this paper, on the basis of the concepts of Gibbs's dividing surface and Rusanov's dividing line, taking the influences of the line tension into account, we thermodynamically investigate the wetting characteristics of cylindrical droplets in a homogeneous and smooth regular triangular prism, which is filled with gas within three apex corners, and derive the corresponding generalized Young equation.

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