4. Molecular Dynamics of Phase-Interface

4.1 Liquid Vapor Interface
- Surface Tension
- Young-Laplace Equation
- Condensation Coefficient

4.2 Liquid-Solid-Vapor Contact
- Liquid Droplet on a Solid Surface
- Vapor Bubble on a Solid Surface
- Contact Angle and Young’s Equation
- Thermal Boundary Resistance between Liquid and Solid

Condensation coefficient $\alpha$

$$\alpha = \frac{\text{Condensation Molecule Flux}}{\text{Incident Molecule Flux}}$$

Matsumoto et al.
Molecular Exchange = Boiling off other molecules
Tsuruta et al.
Connection to DSMC

Young-Laplace Equation

$$\gamma_{li} = \frac{(P_L - P_v)R}{2}$$

$$P_L(r) = k_B T \frac{\nu(r)}{m} \frac{1}{4\pi} \sum_j l_j$$

$$P_v(r) = k_B T \frac{\nu(r)}{m} \frac{1}{4\pi} \sum_j \int l_j \left( \frac{1}{2} \frac{d^2 \nu(r)}{dr^2} \right)$$

Equimolar Dividing Radius

$$mN = \frac{4\pi}{3} R^3 \rho_i + \left( \rho - \frac{4\pi}{3} R^3 \right) \rho_v$$

Tolman Length $\delta$

$$\gamma_{li} = \gamma_{li,0} \left( 1 - \frac{2\delta}{R} \right) + \mathcal{O}(\delta^2)$$

Surface Tension

Surface Tension of Droplet

Condensation Coefficient

Liquid Droplet on Solid Surface
Effect of Potential of Solid-Liquid Molecules

E1: Weaker Interaction  E4: Stronger Interaction

Effect of Temperature

100K 1536 Molecules  130K

50 40 30 20 10 0

Density Profile

Layered Liquid Structure

E1: Weaker Interaction  E4: Stronger Interaction

Effect of Potential of Solid-Liquid Molecules

Layered Liquid Structure
Density and Potential Profiles

Departure of Droplet for $\varepsilon_{\text{SURF}} < 1.0$

Smaller System $\varepsilon_{\text{SURF}} = 1.86$

Density and Potential Profiles

Vapor Bubble on Solid Surface
Snapshots of bubble formation for E3

Two-dimensional density distributions

Contact angle correlated with \( \varepsilon_{\text{SURF}} \)

Definition of contact angle \( \cos \theta \) for E5 and P5

Young’s Equation (Macroscopic)

Thermal Boundary Resistance over Liquid-Solid Interface: \(10^{-7} \text{ – } 10^{-6} \text{ m}^2\text{K/W}\)

Thermal Resistance over Liquid-Solid Interface

Thermal Conductivity
\[ \lambda_v = \frac{q_w}{(\partial T / \partial z)} \]
0.082 W/m K
Handbook value 0.097 W/m K at the saturated temperature of 110 K

Temperature jump: 6.4 K
5.3 K

Temperature vs. Position [Å]

Vapor Solid Liquid Vapor

Solid Liquid Vapor Solid

Contact angle cos \( \theta \)

\[ L \cos \theta \]