

Homework 4 - Solution

Problem 1: Schrage equation

A) Mass balance

Evaluating the mass flux at the interface

i) Emitted molecules from the interface

$$j_s^+ = \int_0^\infty \rho_L f_L v_x dv_x = \int_0^\infty \frac{P_L}{RT_L} \left(\frac{m}{2\pi kT_L} \right)^{\frac{1}{2}} \exp\left(-\frac{mv_x^2}{2kT_L}\right) v_x dv_x$$

ii) Molecules coming from the vapor to the liquid surface

$$j_s^- = \int_{-\infty}^0 \rho_V f_V v_x dv_x = \int_{-\infty}^0 \frac{P_V}{RT_V} \left(\frac{m}{2\pi kT_V} \right)^{\frac{1}{2}} \exp\left(-\frac{m(v_x - u_x)^2}{2kT_V}\right) v_x dv_x$$

Net mass flux is the sum of i) and ii)

$$j_s = j_s^+ + j_s^-$$

Evaluating the mass flux in the far field

$$j_\infty = \int_{-\infty}^\infty \rho_V f_V(v_x) v_x dv_x = \int_{-\infty}^\infty \frac{P_V}{RT_V} \left(\frac{m}{2\pi kT_V} \right)^{\frac{1}{2}} \exp\left(-\frac{m(v_x - u_x)^2}{2kT_V}\right) v_x dv_x$$

Mass flux balance requires

$$j_s = j_\infty$$

So one equation with only v_x as unknown.

$$\begin{aligned} \int_0^\infty \frac{P_L}{RT_L} \left(\frac{m}{2\pi kT_L} \right)^{\frac{1}{2}} \exp\left(-\frac{mv_x^2}{2kT_L}\right) v_x dv_x + \int_{-\infty}^0 \frac{P_V}{RT_V} \left(\frac{m}{2\pi kT_V} \right)^{\frac{1}{2}} \exp\left(-\frac{m(v_x - u_x)^2}{2kT_V}\right) v_x dv_x \\ = \int_{-\infty}^\infty \frac{P_V}{RT_V} \left(\frac{m}{2\pi kT_V} \right)^{\frac{1}{2}} \exp\left(-\frac{m(v_x - u_x)^2}{2kT_V}\right) v_x dv_x \end{aligned}$$

B.1) Momentum balance

Momentum flux in the x-direction evaluated at the liquid-vapor interface

i) At the interface:

$$MF_s = \underbrace{\int_0^\infty \frac{P_L}{RT_L} v_x^2 f_L dv_x}_{\text{outgoing}} + \underbrace{\int_{-\infty}^0 \frac{P_V}{RT_V} v_x^2 f_V dv_x}_{\text{incoming}}$$

ii) In the far field:

$$MF_\infty = \int_{-\infty}^\infty \frac{P_V}{RT_V} v_x^2 f_V dv_x$$

Momentum balance requires

$$\int_0^{\infty} \frac{P_L}{RT_L} v_x^2 f_L dv_x + \int_{-\infty}^0 \frac{P_V}{RT_V} v_x^2 f_V dv_x = \int_{-\infty}^{\infty} \frac{P_V}{RT_V} v_x^2 f_V dv_x$$

B.2) Energy balance

Energy flux at the interface

i) Energy flux associated with the emitted molecules from the interface

$$\int_{-\infty}^{\infty} f_z|_{T=T_L} dv_z \int_{-\infty}^{\infty} f_y|_{T=T_L} dv_y \int_0^{\infty} \frac{1}{2} \frac{P_L}{RT_L} (v_x^2 + v_y^2 + v_z^2) v_x f_L dv_x$$

ii) Energy flux associated with vapor molecules coming back to the interface

$$\int_{-\infty}^{\infty} f_z|_{T=T_V} dv_z \int_{-\infty}^{\infty} f_y|_{T=T_V} dv_y \int_{-\infty}^0 \frac{1}{2} \frac{P_V}{RT_V} (v_x^2 + v_y^2 + v_z^2) v_x f_V dv_x$$

Energy flux evaluated in the far field

$$\int_{-\infty}^{\infty} f_z|_{T=T_V} dv_z \int_{-\infty}^{\infty} f_y|_{T=T_V} dv_y \int_{-\infty}^{\infty} \frac{1}{2} \frac{P_V}{RT_V} (v_x^2 + v_y^2 + v_z^2) v_x f_V dv_x$$

Energy balance requires

$$\begin{aligned} & \int_{-\infty}^{\infty} f_z|_{T=T_L} dv_z \int_{-\infty}^{\infty} f_y|_{T=T_L} dv_y \int_0^{\infty} \frac{1}{2} \frac{P_L}{RT_L} (v_x^2 + v_y^2 + v_z^2) v_x f_L dv_x \\ & + \int_{-\infty}^{\infty} f_z|_{T=T_V} dv_z \int_{-\infty}^{\infty} f_y|_{T=T_V} dv_y \int_{-\infty}^0 \frac{1}{2} \frac{P_V}{RT_V} (v_x^2 + v_y^2 + v_z^2) v_x f_V dv_x \\ & = \int_{-\infty}^{\infty} f_z|_{T=T_V} dv_z \int_{-\infty}^{\infty} f_y|_{T=T_V} dv_y \int_{-\infty}^{\infty} \frac{1}{2} \frac{P_V}{RT_V} (v_x^2 + v_y^2 + v_z^2) v_x f_V dv_x \end{aligned}$$

Problem 2: Simulating evaporating sessile droplet

For $h = 0.2\text{mm}$, the evaporation mass flux is larger toward the edge and smaller near the center. Applying the symmetry (Figure 2), one can see that the edge corresponds to a small radius of curvature. This is where you expect to find larger concentration gradients on the boundary when solving a Laplace equation (analogous to the lightning rod problem in the context of Maxwell equations).

When $h = 1\text{mm}$, the droplet is a hemi-sphere. Applying the same symmetry operation, you would find that the curvature is constant along the liquid surface from the center to the edge. Therefore, in the plot, the evaporation mass flux is constant.

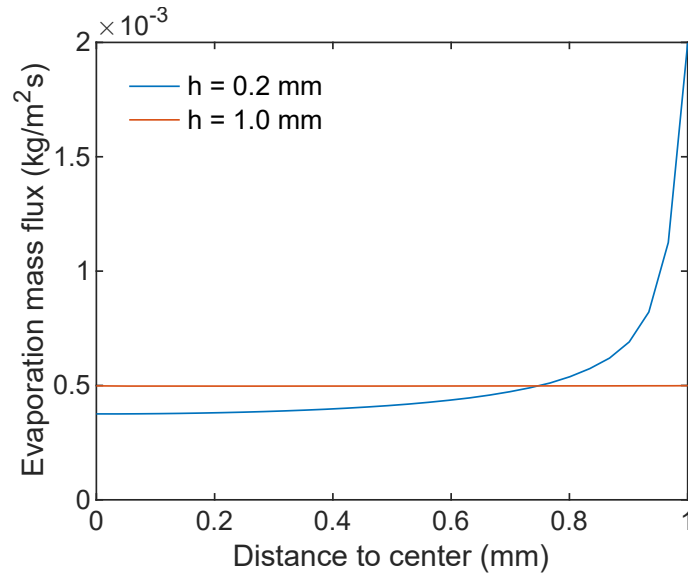


Figure 1: Evaporative mass flux as a function of the r -coordinate for droplet height $h = 0.2\text{mm}$ and $h = 1\text{mm}$.

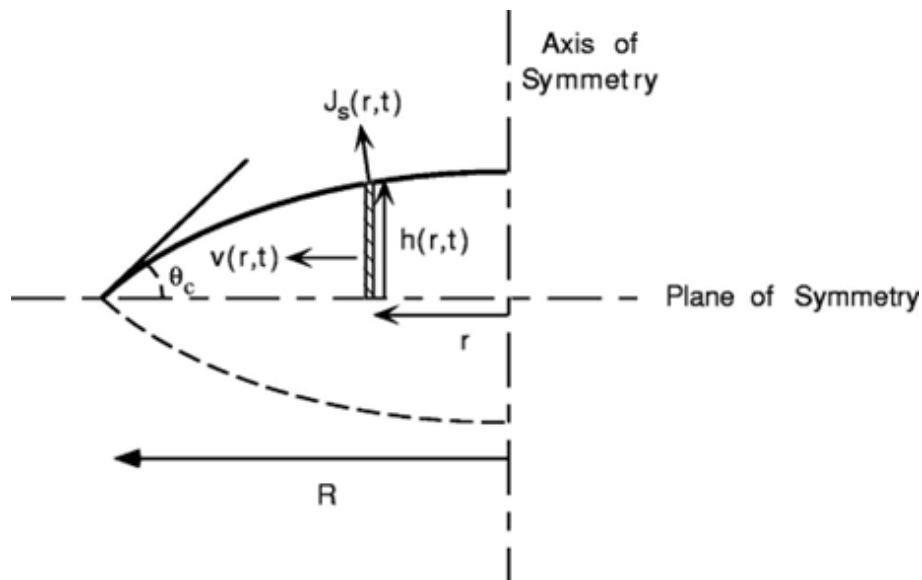


Figure 2: Axisymmetric model of a sessile droplet evaporation.

Problem 3: Average kinetic energy

Beginning with the expression for \bar{e}_k :

$$\bar{e}_k = \int f \frac{m}{2} (u^2 + v^2 + w^2) dudvdw$$

Substituting the expression for u , v and w in terms of the relative velocities

$$\bar{e}_k = \int f \frac{m}{2} (u_r^2 + 2u_r u_0 + u_0^2 + v_r^2 + 2v_r v_0 + v_0^2 + w_r^2 + 2w_r w_0 + w_0^2) dudvdw$$

Now, we can separate it into three parts:

$$\begin{aligned} \bar{e}_k &= \int f \frac{m}{2} (u_r^2 + v_r^2 + w_r^2) dudvdw \\ &\quad + \int f \frac{m}{2} (2u_r u_0 + 2v_r v_0 + 2w_r w_0) dudvdw + \frac{m}{2} (u_0^2 + v_0^2 + w_0^2) \int f dudvdw \end{aligned}$$

By definition, we know that the integral of the velocity distribution function over all possible velocity is equal to 1:

$$\int f(u, v, w) dudvdw = 1$$

Analyzing the cross terms. Since u_0 , v_0 , and w_0 are constants (bulk velocities), we can factor them out of the integrals. This leaves us with:

$$\frac{m}{2} \left(2u_0 \int f u_r dudvdw + 2v_0 \int f v_r dudvdw + 2w_0 \int f w_r dudvdw \right)$$

By definition, u_r , v_r , and w_r are deviations from the bulk velocities. Therefore, their averages is null:

$$\int f u_r dudvdw = \int f v_r dudvdw = \int f w_r dudvdw = 0$$

Thus the cross term is null and we obtain:

$$\bar{e}_k = \bar{e}_{kr} + e_{kb}$$

with

$$\bar{e}_{kr} = \int f \frac{m}{2} (u_r^2 + v_r^2 + w_r^2) dudvdw$$

and

$$e_{kb} = \frac{m}{2} (u_0^2 + v_0^2 + w_0^2)$$