

Homework 4

Presentation by Group 4 on Thursday 9th October

Problem 1: Schrage equation

Consider the half-space evaporation problem for a single-component system, assuming that the condensation coefficient = 1. At the liquid surface, the temperature is T_L and the vapor pressure is the saturation vapor pressure at that temperature, P_L . Here, we know the velocity distribution function of molecules emitted from the surface takes a half-Maxwellian form:

$$f_L|_{v_x>0}dv_x = \left(\frac{m}{2\pi kT_L}\right)^{\frac{1}{2}} \exp\left(\frac{-mv_x^2}{2kT_L}\right) dv_x$$

where m is the mass of one vapor molecule.

In the far-field vapor, the temperature T_V and the pressure P_V can also be measured. The velocity distribution is a drifted Maxwell-Boltzmann distribution:

$$f_V dv_x = \left(\frac{m}{2\pi kT_V}\right)^{\frac{1}{2}} \exp\left(\frac{-m(v_x - u_x)^2}{2kT_V}\right) dv_x$$

with u_x being the unknown bulk vapor velocity in the far field.

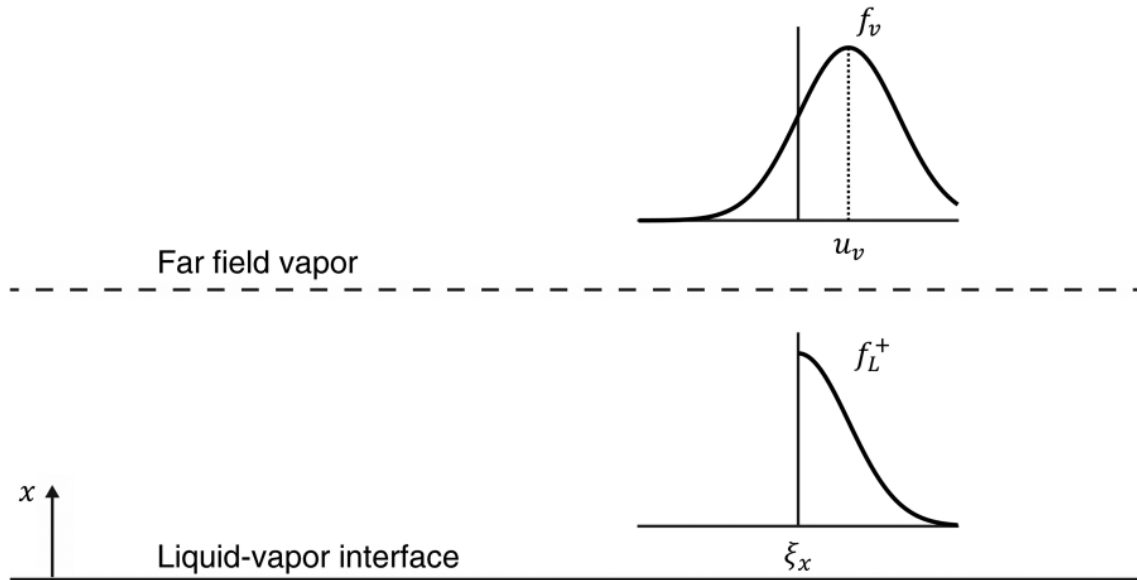


Figure 1: Marginal velocity distribution in x on an evaporating surface and in the far-field vapor. For the surface, we are only showing the positive half of the distribution. (DOI: 10.1115/1.4054382)

To formulate the conservation equation, Schrage assumed in his thesis that

$$f_L|_{v_x < 0} dv_x = f_V|_{v_x < 0} dv_x$$

and the mass flux for the backflowing vapor molecules is:

$$j_s^- = \int_{-\infty}^0 \frac{P_V}{RT} f_V v_x dv_x$$

A) With the help of the ideal gas law, write down the mass balance equation between the surface and the far field. You don't have to carry out the integrals. *Conclude that you can solve for the only unknown in this equation (u_x).*

B) Write down momentum balance and the energy balance (assuming the gas molecules only carry the translational kinetic energy) after reading the note below. Assume the velocity distribution in the y - and z -direction follows the symmetric Maxwell-Boltzmann distribution characterized by local temperature:

$$f_y dv_y = \left(\frac{m}{2\pi kT} \right)^{\frac{1}{2}} \exp\left(\frac{-mv_y^2}{2kT} \right)$$

$$f_z dv_z = \left(\frac{m}{2\pi kT} \right)^{\frac{1}{2}} \exp\left(\frac{-mv_z^2}{2kT} \right)$$

You don't have to carry out the integrals. *From this problem, you can see Schrage's assumption over-constrains the problem as we have three independent equations for one unknown u_x .*

Note: For a general separable velocity distribution function $f(v_x, v_y, v_z) = f_x f_y f_z$ with a local density ρ , the momentum flux in the x -direction at the surface can be calculated as follows.

If the vapor molecules at a certain location have the velocity v_x in the x -direction, the x -direction momentum flux is then $\rho v_x \cdot v_x$, where the first part is the momentum carried by the molecules (per unit volume) and the second part gives us the rate at which the molecules are entering the boundary (velocity normal to the boundary can be seen as the volume flux). The probability that this occurs is $f_x dv_x$. Therefore, the actual momentum flux is the expectation value of $\rho v_x \cdot v_x$.

$$MF = \int \rho v_x \cdot v_x f_x dv_x$$

If the distribution f and the effective density ρ is not continuous at $v_x = 0$ (as in the case of Schrage's assumption for the interface), one can also write

$$MF = \int_{-\infty}^0 (\rho v_x \cdot v_x f_x)|_{v_x < 0} dv_x + \int_0^{\infty} (\rho v_x \cdot v_x f_x)|_{v_x > 0} dv_x$$

For the energy flux, if the vapor molecules at a certain location have the velocity vector (v_x, v_y, v_z) , the x -direction kinetic energy flux is then $\frac{1}{2} \rho (v_x^2 + v_y^2 + v_z^2) \cdot v_x$, where the first part is the total kinetic energy carried by the molecules (per unit volume) and the second part gives us the rate at which the molecules are entering the boundary. The probability that this occurs is $f_x dv_x f_y dv_y f_z dv_z$ (we need to consider the y and the z directions because the kinetic energy contains v_y and v_z terms).

Therefore, the actual energy flux is the expectation value of $\frac{1}{2}\rho(v_x^2 + v_y^2 + v_z^2) \cdot v_x$.

$$EF = \int f_z dv_z \int f_y dv_y \int \frac{1}{2}\rho(v_x^2 + v_y^2 + v_z^2) \cdot v_x f_x dv_x$$

If the distribution f and the effective density ρ is not continuous at $v_x = 0$ (as in the case of Schrage's assumption for the interface), one can also write

$$EF = \int f_z dv_z \int f_y dv_y \int_{-\infty}^0 \left[\frac{1}{2}\rho(v_x^2 + v_y^2 + v_z^2) \cdot v_x f_x \right]_{v_x < 0} dv_x \\ + \int f_z dv_z \int f_y dv_y \int_0^{\infty} \left[\frac{1}{2}\rho(v_x^2 + v_y^2 + v_z^2) \cdot v_x f_x \right]_{v_x > 0} dv_x$$

Problem 2: Simulating evaporating sessile droplet

Carefully read the *Matlab* code we uploaded for evaporation from a sessile droplet. The presenter of this question should briefly explain what each part of the code does.

Modify the code to plot the **evaporative mass flux distribution** along the droplet surface as a function of the r-coordinate (distance to the center line) for droplet height $h_1 = 0.2mm$ and $h_2 = 1.0mm$ (while fixing everything else) on the same figure.

Explain the different trend you observe for the two cases (considering the lightening rod analogy and the symmetry in the simulation domain).

Problem 3: Average kinetic energy

Following the lecture's nomenclature, if we know the average kinetic energy of a molecule is defined as

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

Define the relative velocity of a molecule as u_r , v_r , and w_r in the x , y , z directions as

$$u_r = u - u_0; \quad v_r = v - v_0; \quad w_r = w - w_0$$

where u_0 , v_0 , w_0 are the bulk average velocity in the x , y , z directions.

Show that

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

where

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

and

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