Homework Assignment 2

Interfacial Transport Phenomena

Due date: 02.Apr.2024

In this homework assignment, we will solve several questions involving interfacial transport phenomena that can be answered based on our knowledge from Lectures 3 - 6.

Q1 Meniscus Profile Adjacent to a Wilhelmy Plate

In Lecture 4, we have shown that the governing equation for the meniscus profile adjacent to a Wilhelmy plate is given by:

$$\frac{\mathrm{d}^2 H}{\mathrm{d}X^2} = \mathrm{Bo} \times \left\{ H \left[1 + \left(\frac{\mathrm{d}H}{\mathrm{d}X} \right)^2 \right]^{3/2} \right\} \tag{1}$$

with boundary conditions:

$$\begin{cases} \frac{\mathrm{d}H}{\mathrm{d}X}(X=0) = -\cot\theta \\ H(X \to \infty) = \frac{\mathrm{d}H}{\mathrm{d}X}(X \to \infty) = 0 \end{cases} \tag{2}$$

where $H = h/l$, $X = x/l$ are the dimensionless height and distance away from the surface, respectively. l is the characteristic length scale of the system. $\mathrm{Bo} = \rho g l^2/\gamma$ is the Bond number. In other words, when the length scale $l = \sqrt{\frac{\gamma}{\rho g}}$ is used, $\mathrm{Bo} = 1$, we will use this condition in all the questions.

Please answer the following questions:

1. When $\theta > 90°$, is the pressure on the liquid side near the plate higher or lower than 1 atm?

2. Write a function f that:

   - **Input**: contact angle θ, initial height $H_0 = H(X = 0)$ and value(s) of X
   - **Output**: value(s) of H and $\frac{\mathrm{d}H}{\mathrm{d}X}$ depending on the input of X

   You may use any numerical tool for differential equations, for instance the Runge-Kutta methods `ode45` implemented in Matlab.

3. We will first try to solve the differential equation numerically. To do so we have to use an initial guess for H_0 to be inserted into f. To find the correct value for H_0 with contact angle θ, we can check if both $H(X \to \infty) = 0$ and $\frac{\mathrm{d}H}{\mathrm{d}X}(X \to \infty) = 0$ are met. To

simplify the problem, we only examine the value at a finite X value that is large enough (for instance $X = 3$).

Assume $\theta = 45°$, plot the values of $H(X = 3)$ and $\frac{\mathrm{d}H}{\mathrm{d}X}(X = 3)$ as functions of your initial guess of H_0 within the range $0 \leq H_0 \leq 1$, respectively. Which H_0 will meet the boundary conditions? Comment on the sensitivity of the ODE equations on the choice of H_0.

4. With your knowledge in Q1.3, write a numerical procedure to solve the value of H_0, given the contact angle θ. Plot the value of H_0 as a function of θ for $0° \leq \theta \leq 180°$. (Cation: root-finding algorithms like `fsolve` in Matlab will only give reasonable solution if your choice of H_0 is close enough to the exact solution! Avoid using 0 and 1 for H_0.)

5. Plot the H - X profiles of the meniscus for the following cases:

   - $\theta = 20°$
   - $\theta = 75°$
   - $\theta = 150°$

   Your solutions should at least work for the ranges $0 \leq X \leq 3$.

   (Bonus) Optimize your code and push the upper limit of X to $X = 5$ or even $X = 10$. Describe how you achieve this.

6. Due to the complexity of formulation, the analytical solution for the differential equation is expressed as function $X(H)$ rather than $H(X)$ and is known as,

$$X - X_0 = \operatorname{arccosh}\left(\frac{2}{H}\right) - 2\sqrt{1 - \frac{H^2}{4}} \tag{3}$$

   for menisci with $H > 0$, whereas X_0 is the offset so that H reaches its initial height at the wall for $X = 0$. Plot and compare your results from Q1.5 for $\theta = 20°$ and $75°$ with the analytical solution. You can do this by using your calculated values for H to get the corresponding positions X. Please comment your results from the comparison.

   (Cation: Don't forget to consider the offset X_0 which in your case is equal to the calculated value for X using the first height H from your results from Q1.3)

Q2 Growth of Ice Crystal in Salt Water

We consider a salt water bath, with uniform salt concentration $C = C_\infty$ and temperature $T = T_\infty$, before putting in an ice seed. As you know, salt lowers the equilibrium freezing temperature of the solution, T_F, following $T_F = T_0 - \beta C_{IL}$, where T_0 is the freezing temperature of pure water, β is a positive constant (known), and C_{IL} is the interface salt concentration on the liquid side. Here we assume the grown ice crystal does not contain any salt (i.e., $C_{IS} = 0$). Now we carefully put a small spherical ice seed in the middle of the bath, and then the growth begins. The ice crystal is assmued to be perfectly spherical, with its radius $a(t)$ increasing as a function of time t. Please answer the following questions:

1. During growth, do you expect to see $C_{IL} > C_\infty$ or $C_{IL} < C_\infty$? Why? (3%)
2. Using the interface heat balance and under the assumption that the ice seed temperature is T_0, please express the ice growth rate $\frac{da}{dt}$, using the thermal conductivity of liquid water k_L, the interface temperature T_I, the density of liquid water ρ_L, the latent heat per unit mass λ and the radius a, by assuming that the densities of solution and ice are identical.
3. Using the interface mass transfer balance, please express the interface concentration on the liquid side C_{IL}, using C_∞, a, the salt diffusivity in liquid water D_L, and the growth rate $\frac{da}{dt}$. Note that we assume $C_{IS} = 0$.
4. In combination of the fact that $T_I = T_F = T_0 - \beta C_{IL}$, together with the expressions you obtained in Q2.2. and Q2.3., please show the final equations you will have to solve in order to obtain $a(t)$. Its suffcient to write them down, you don't need to solve it.