CH620003 Process Modelling and Simulation

Assignment 4 Deadline to submit: **01 May 2025 (before 12 noon)**

Q1. Problem on finite difference scheme: Heating in micro-electronic circuits

The Fourier heat conduction equation in 1D space is

$$\frac{\partial}{\partial t}(\rho c_p T) = \frac{\partial}{\partial x}\left[k(T)\frac{\partial T}{\partial x}\right]$$

where $k(T)$ is the temperature dependent thermal conductivity of SILVER. You can use any available resource to find out the $k(T)$, either regressing (polynomial fit) the temperature versus thermal conductivity data, or using a mathematical relationship. But remember $k(T)$ is not $constant$ and should be considered to be function of T.

Consider the density ρ and specific heat capacity c_p as constant, for SILVER. Please find these values from some resource (e.g. google / perry's handbook / etc.)

The initial and boundary conditions are-

at $t = 0, T = T_0 = 300\ K$ and at $x = 0, T = T_0[1 + \sin(2\pi\omega t)]$

where ω is the frequency of the fluctuation. The temperature at one end of the domain follows a sinusoidal variation. This particular problem is relevant in heating of electric-vehicle charging ports connected to an AC source. You can relate the ω to be frequency of the AC supply.

at $x = L = 1cm, T = T_0$ (constant temperature)

Calculate the temperature profile $T(x = 0.25L, t)$, $T(x = 0.5L, t)$, $T(x = 0.75L, t)$ and $T(x = L, t)$ using **(a)** Explicit and **(b)** Implicit finite difference numerical scheme, and **(c)** Crank Nicholsan method. You need to calculate the temperature profile for at least 5 cycles of ω. For e.g., if $\omega = 1$ Hz, you need to calculate for the final time up to 5s; for $\omega = 50\ Hz$, final time should be computed up to 100 ms.

Note for the explicit scheme, you need to take care of the Von-Neumann stability criterion.

(d) Using the explicit scheme, change the parameter $\lambda = \frac{\alpha \Delta t}{(\Delta x)^2}$ to check the numerical convergence. Show how the solution behaves when λ exceeds the von-Neumann stability criteria.

Compare the explicit results with the implicit scheme, in terms of accuracy of the solution.

(e) Change the number of internal grid points from 10 to 1000 to 10^5, and estimate the computational time needed to solve the tri-diagonal matrix (TDM) in the Implicit scheme using classical matrix inversion techniques (gauss-elimination, gauss-Jordan, gauss-newton, etc.) vis-à-vis the Thomas algorithm.

(f) Plot $T(x = 0, t)$ and length averaged $\bar{T}(t) = \frac{1}{L}\int_0^L T(x,t)\ \mathrm{d}x$ with t, for different values of of ω. Is there any phase difference observed between the average temperature response, with respect to $x = 0$.

Determine the critical value of ω, beyond which the temperature variations at the other tip $[T(x = L, t)]$ is minimal. Does this critical value of ω depend on α ? Support your answer with results.

Q2. Bubble dynamics – combustion engineering

When an insoluble bubble rises in a deep pool of liquid, its volume increases according to the ideal gas law. However, when a soluble bubble rises from deep submersion, there is a competing action of dissolution that tends to reduce size. Under practical conditions, it has been proved that the mass transfer coefficient (k_c) for spherical particles (or bubbles) in free-fall (or free-rise) is substantially constant. Thus, for sparingly soluble bubbles released from rest, the following material balance is applicable,

$$\frac{d}{dt}\left(c\,\frac{4}{3}\pi R^3\right) = -k_c\; 4\pi R^2(t)\;\; c^*$$

where c is the ideal gas molar density, c^* is molar solubility of gas in liquid and $R(t)$ is the changing bubble radius. The pressure at a distance z from the top liquid surface is $P = P_A + p_L g z$ and the rise velocity is assumed to be quasi-steady and follows the intermediate law to give a linear relation between speed and size,

$$\frac{dz}{dt} = 2\left(\frac{2g}{15\,\nu^{1/2}}\right)^{\frac{2}{3}} R(t) = \beta\, R(t)$$

where ν is the kinematic viscosity of the liquid and g is the gravitational acceleration.

(a) Derive a differential equation that relates the bubble radius $R(t)$ with the pressure P.

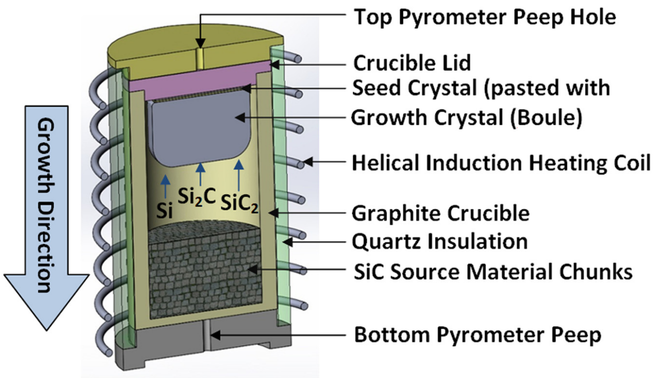
(b) Solve the differential equation subject to the initial condition, $R(0) = R_0$ and $P(0) = P_0 = P_A + \rho_L g z_0$. Also find the time (or depth) at which the soluble bubble completely disappears, $R \to 0$.

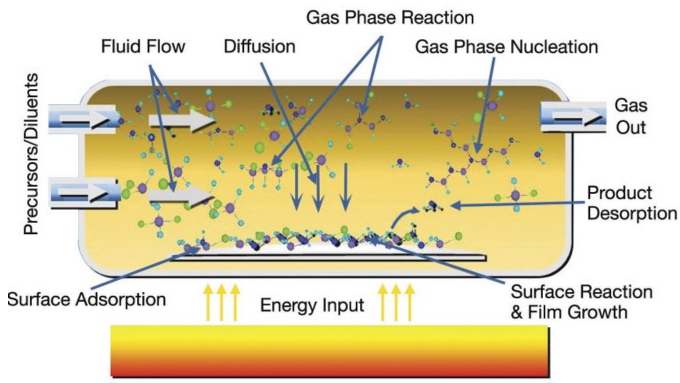
Q3. Crystal shape / size evolution in vapour phase condensation – semiconductor manufacturing

During physical vapour deposition (PVD) process, there is deposition of gas phase molecules over the seed surface by crystallization, leading to the formation of high quality (single) crystals generally. In chemical vapour deposition (CVD), there is reaction of gaseous molecules on solid substrate leading to formation or growth of a thin layer. During the PVD, there is fluid, heat and mass transport followed by crystallisation, whereas in CVD it is mostly mass transport and chemical reaction. Since, these processes involve working with metallic vapours, the temperature range is usually very high above the boiling point of metals and operated at low pressures.

One the typical examples of PVD is the production of Silicon (single) crystals which is used as a electronic material in p-n diodes, transistors, microprocessors, etc.

CVD is generally used to prepare nanomaterials –single layered graphene nanotube, novel photo-adsorbents, etc. and artificial diamonds!





[Left] Physical vapour transport process in bulk crystal growth; [Right] Chemical vapour deposition process.

Develop a detailed mathematical model for the evolution of the crystal growth (for PVD) or thin film growth (for CVD) given that you know the temperature field in the reactor. Note that you need to consider heat transfer inside the crystal material (and the thickness will grow in time) as it is thermally conductive.

You DO NOT need to solve the model for this problem, only the mathematical model is to be formulated.

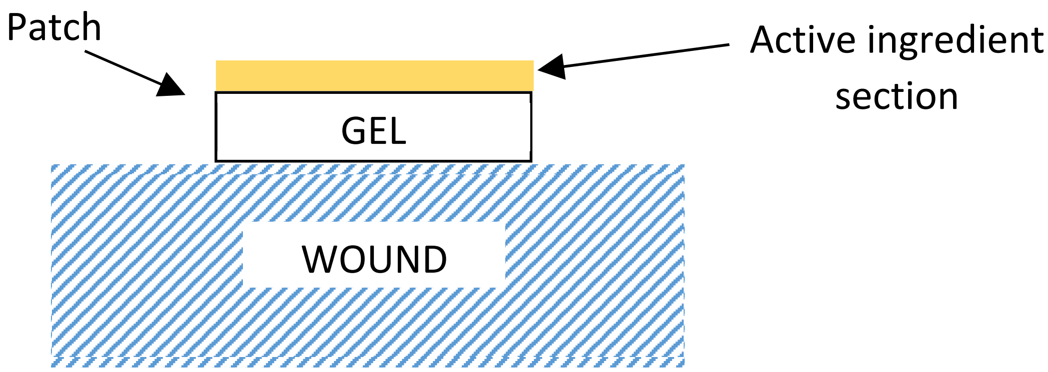
Q4. Wearable tech (Skin patch for drug release)

A pharmaceutical company recently patented a new drug patch to treat a skin wound. The idea of this patch is to release a constant rate of active ingredient to the wound, and to achieve this goal, the manufacturer developed the patch as a two-layer material. One layer that is adjacent to the skin is a gel layer, which is designed to control the rate of release of active ingredient, while the top layer is loaded with active ingredient. The gel layer is the layer through which the active ingredient must diffuse to reach the skin, where the active ingredient is instantly consumed.

Develop a mathematical model for this process technology and compute the dynamics of the concentration profile.

Once the patch is applied onto the wound, how long does it take before the active ingredient reaches the skin and becomes effective? This will let the medical personnel know how long it takes for the patch to start to become effective in the treatment. The effective concentration in this instance is taken to be 0.5% of the concentration of the active ingredient in the top layer.

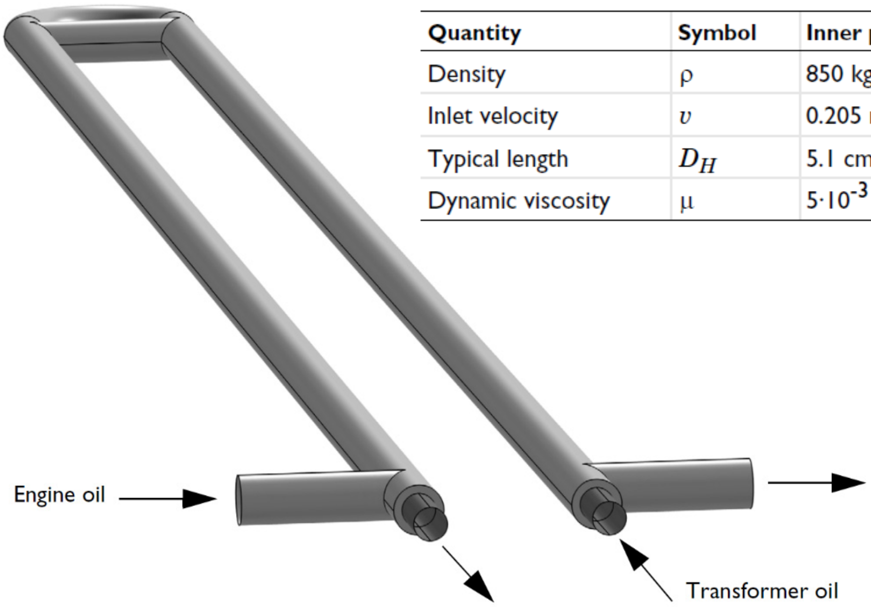
If the quantity of the active ingredient is M, find an expression to determine the time taken to consume all the active ingredients. This will let the medical personnel know the time to replace the patch.



Q5. Double Pipe Heat Exchanger

Double-pipe heat exchangers, with their typical U-turn shape, are one of the simplest and cheapest type of heat exchangers used in the chemical process industry.

Quantity	Symbol	Inner pipe	Outer pipe
Density	ρ	850 kg/m^3	825 kg/m^3
Inlet velocity	v	0.205 m/s	0.09 m/s
Typical length	D_H	5.1 cm	1.3 cm
Dynamic viscosity	μ	$5 \cdot 10^{-3}$ Pa·s	$1 \cdot 10^{-3}$ Pa·s

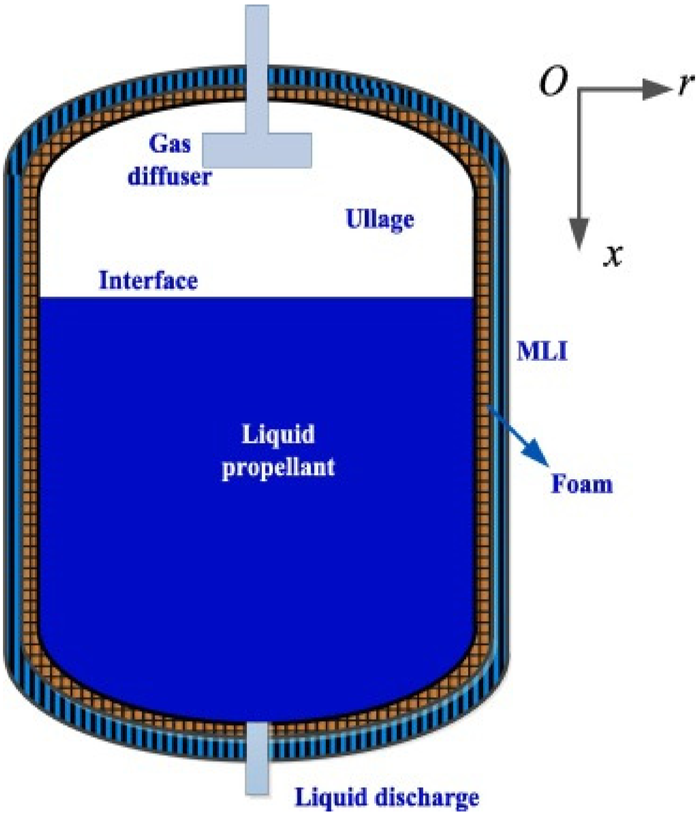


The heat exchanger is made of high tensile steel (Steel AISI 4340). The radii of the concentric pipes are 10 cm and 25 cm, while the overall length is about 6 m. Engine oil at 130°C flows through the outer pipe and is cooled by a transformer oil at 60°C, flowing in counter-current through the inner pipe to prevent the engine oil from Engine oil overheating. The exterior surface of the outer tube is exposed to ambient atmosphere with natural air convection.

Numerically, simulate this system and obtain the temperature profile along the length of the pipe and along the radius.

Q6. Hydrogen Tank: storage conditions

The heat transfer and phase change processes of cryogenic liquid hydrogen (LH2) in the tank have an important influence on the working performance of the liquid hydrogen-liquid oxygen storage and supply system of rockets and spacecrafts. A super critical spherical storage system with double walled tank for hydrogen is to be developed for space environment. During the outflow of the propellant, the pressure inside the storage tank will be maintained above critical pressure using electrical heaters. Propellant is expected to transit from trans-critical to super critical state during operation. Model should include all modes of heat transfer from space environment to the storage fluid.



The evolution of pressure and temperature is to be estimated for the following scenarios.

* During ground servicing in gravity field.

* During operational condition in microgravity field with & without fluid outflow (for different flow rates depending on consumption).

* Estimation of minimum flow rate required to avoid tank venting for different heat in leak conditions.

* Estimation of various modes of heat transfer

* Thermal stratification inside the storage system.

* Evolution of pressure and temperature.

* Heater power requirement for maintaining tank pressure above critical value.