INDIAN INSTITUTE OF TECHNOLOGY KANPUR

DEPARTMENT OF CHEMICAL ENGINEERING

CHEMINEERS SOCIETY

SIMUTECH PROJECT

Submitted by

GROUP - B

PROJECT On

Chemical Engineering Applications: Process, Modelling and Design

(ChEA: PMD)

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WORK DISTRIBUTION

S.no.	Name	Part contributed to
1.	ADITYA KUSHWAHA	Task 1 Implementation Model
2.	PRATEEK KUMAR PANDEY	Task 2 Recapitulation
3.	PRATYUSH GUPTA	Task 2 Optimization Task 1 Simplified Model Task 1 Implementation Model
4.	ANIRUDH SHARMA	Initial Formulation of Task 1 Simplified Model

TASK 1

SIMPLIFIED MODEL

Objective: To analyse a rectangular unifin model using finite element method at transient state.

Given data:

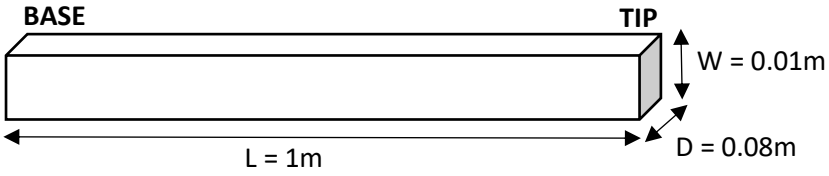
- Isotropic thermal conductivity, k = 200 W/(m.deg C)
- Medium density, ρ = 3000 kg/m^3
- Specific heat, C = 200 J/(kg.deg C)
- Initial temperature T_o uniform throughout the base and is always maintained at 50 deg C.
- Initial temperature (t=0) around fin tip was estimated to be around 20 deg C.
- Convective coefficient of medium, h = 2.5 W/(m^2.deg C)
- Ambient temperature, T_A = 25.8 deg C

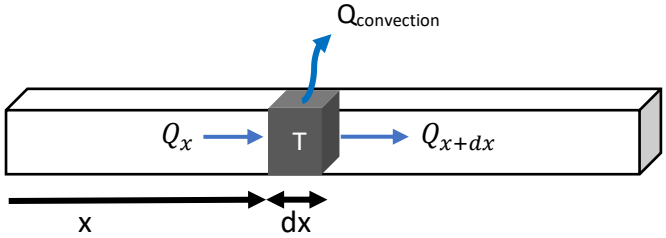
Important points to consider:

- Algebraic method (explicit) to be used
- Finite element method to be used
- 1D transient state
- Using appropriate assumptions to apply Newton's Law of Cooling and Fourier's Law of Conduction

To report:

- Temperature profile w.r.t fin length at t = 0 min, 2 mins, 10 mins, 15 mins and 20 mins.
- The optimised fin length





Q_x and **Q_{x+dx}** represent heat transfer rate by conduction through the cross sections at x and x+dx of the small element

$Q_{convection}$ represent heat transfer rate by convection from the lateral surface of the small element

Applying **General Heat Balance** equation for the small element –

$$\mathbf{Q_x = Q_{x+dx} + Q_{convection} + \rho C \frac{\partial T}{\partial t}} \quad \text{, at transient state } \rho C \frac{\partial T}{\partial t} \neq 0$$

Using Newton's Law of Cooling and Fourier's Law of Conduction, we get the following differential equation –

$$\mathbf{c_1 * \frac{\partial T}{\partial t} + c_3 * \frac{\partial^2 T}{\partial x^2} + c3 * (T - T_A) = 0}$$

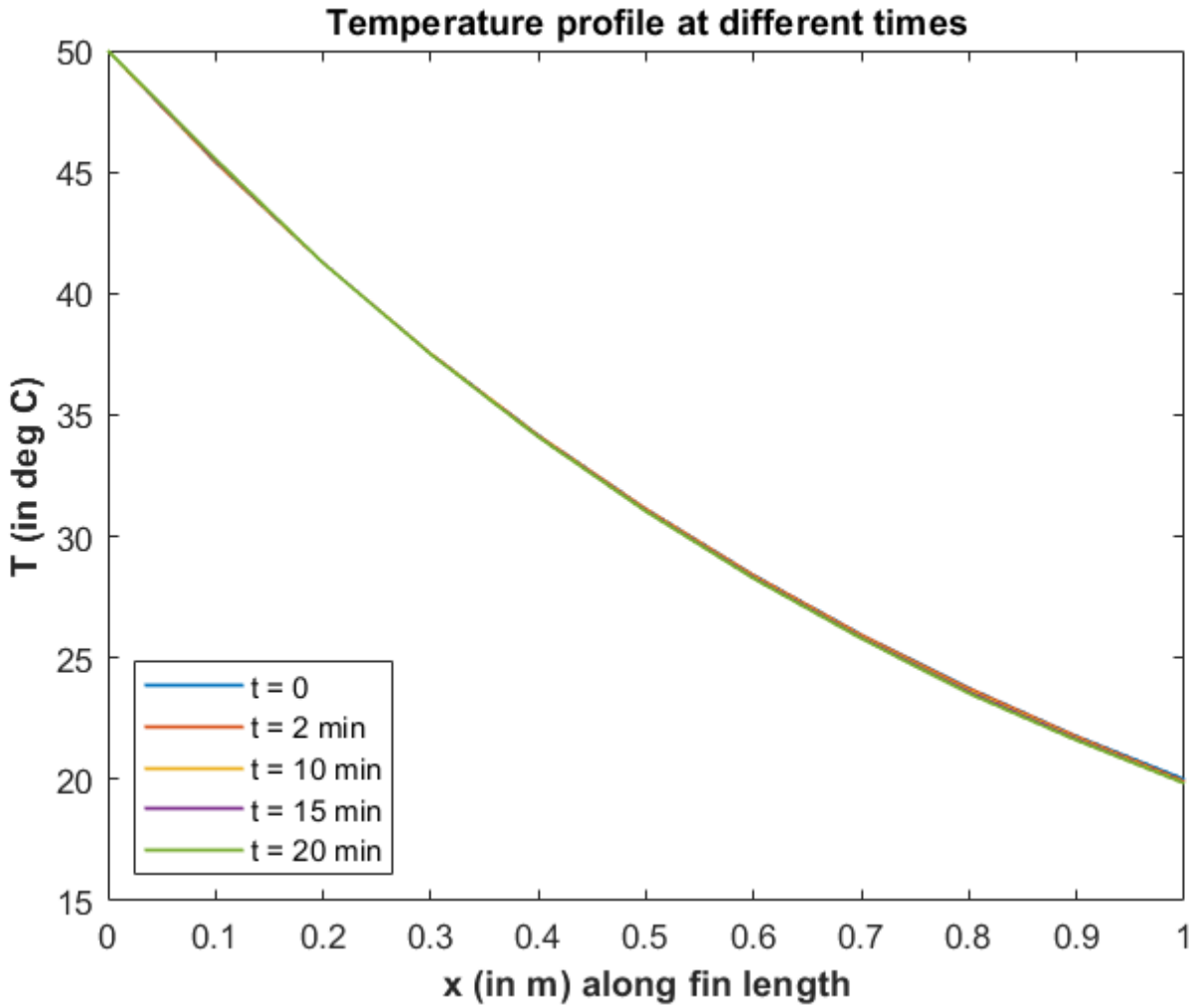
where,

$c_1 = \rho CWD$

$c_2 = -kWD$

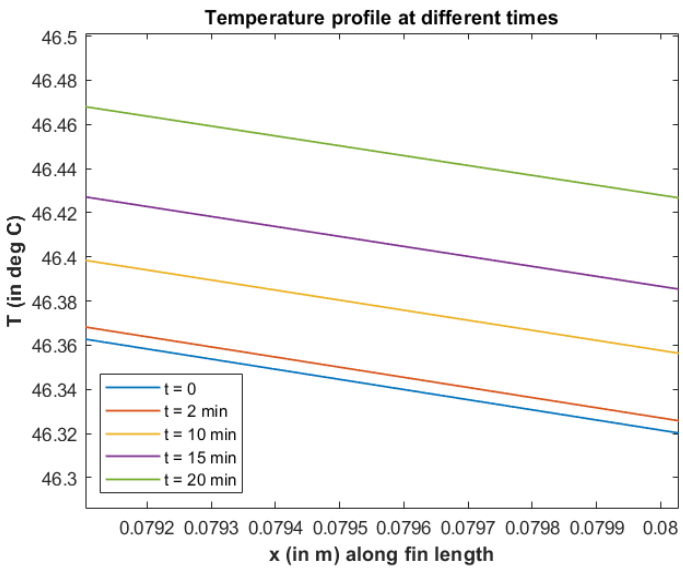
$c_3 = 2h(D + W)$

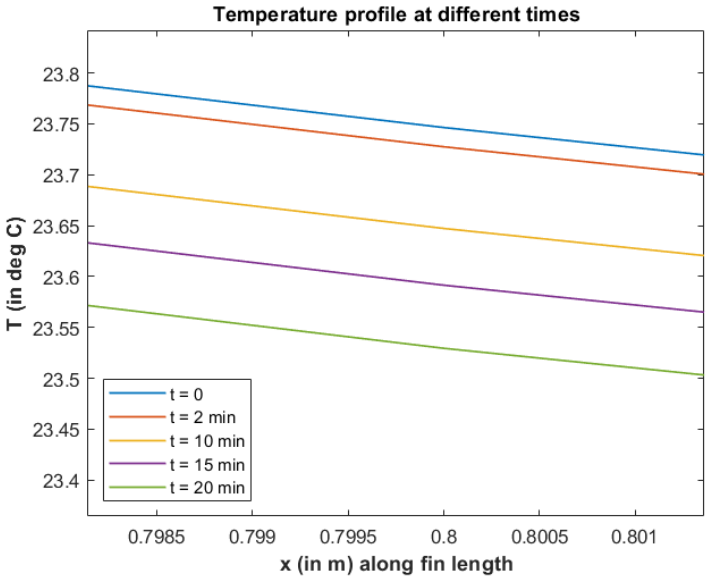
Now, approximating the single and the double derivative by forward and central difference approach and using iterative process, we were able to obtain the following temperature profiles in MATLAB –



Note: They may seem the same plot but if we zoom-in, we can see that the plots don't actually coincide.

On zooming in-





We can see that the relative order of the temperature profiles at different time instants is different at the starting (x~0) and ending stages (x~1).

A possible reason for the initial higher temperature (graph 1 above) for profiles at later time instants can be the fact that initially, the fin tip temperature (20 deg C) is less than the ambient temperature (25.8 deg C). Hence some heat will flow from the surrounding to the fin resulting in the formation of heat junctions with higher temperature than what was at t = 0.

Optimised length at steady state is the distance along the fin length at which $T \sim T_A$. It is observed that the extra length left after the optimised length is of little help and only increases the cost.

From the temperature profiles obtained for the question, we get the optimised fin length to be around **0.7m** and the steady state is obtained sometime between **18 to 20 minutes**.

IMPLEMENTATION MODEL

Objective: To implement a rectangular multi-fin model at steady state in COMSOL.

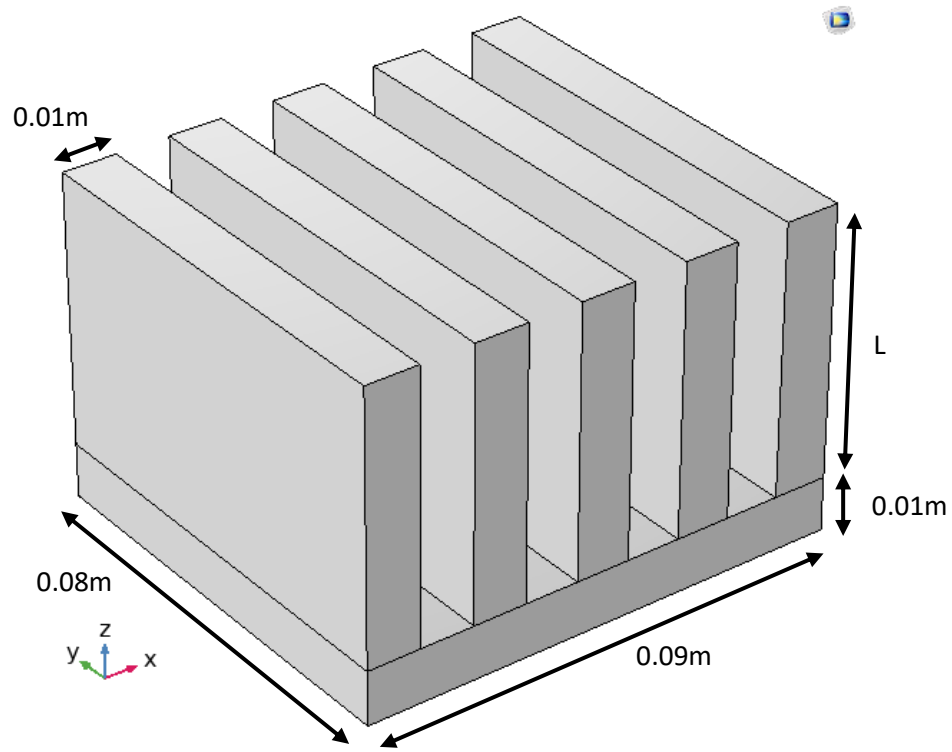
Given data:

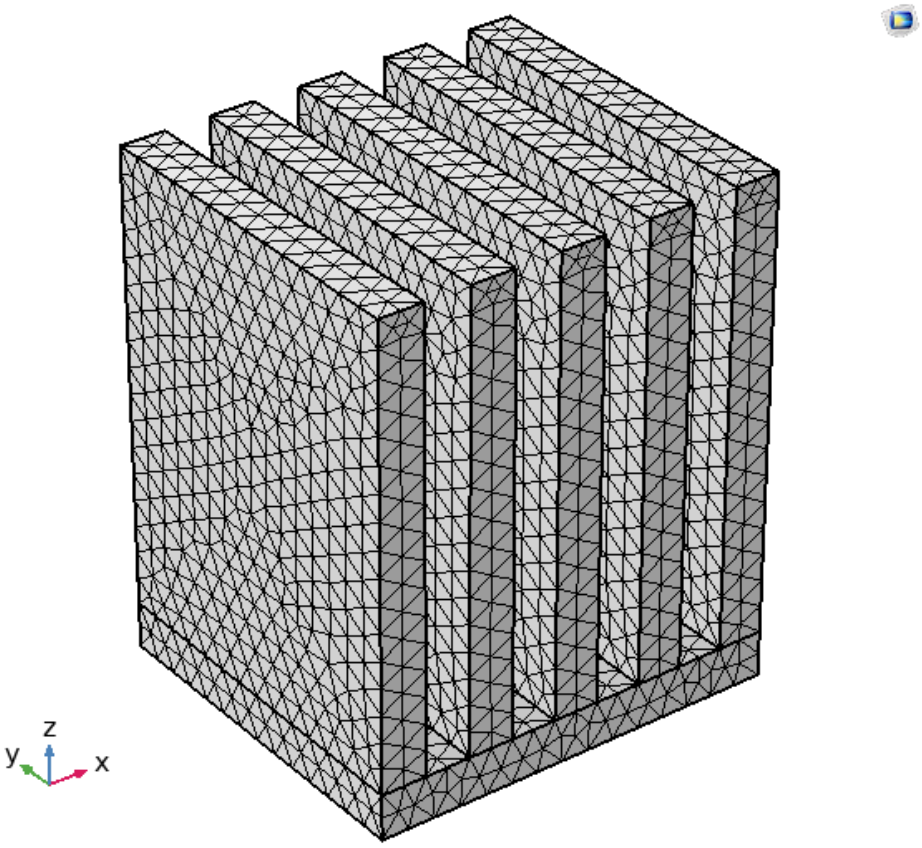
- Material: Copper
- Initial temperature T_O is uniform throughout the base and is always maintained at 50 deg C.
- Convective coefficient 'h' of medium = 2.5 W/(m^2.deg C)
- Ambient Temperature T_A = 25.8 deg C

COMSOL configuration:

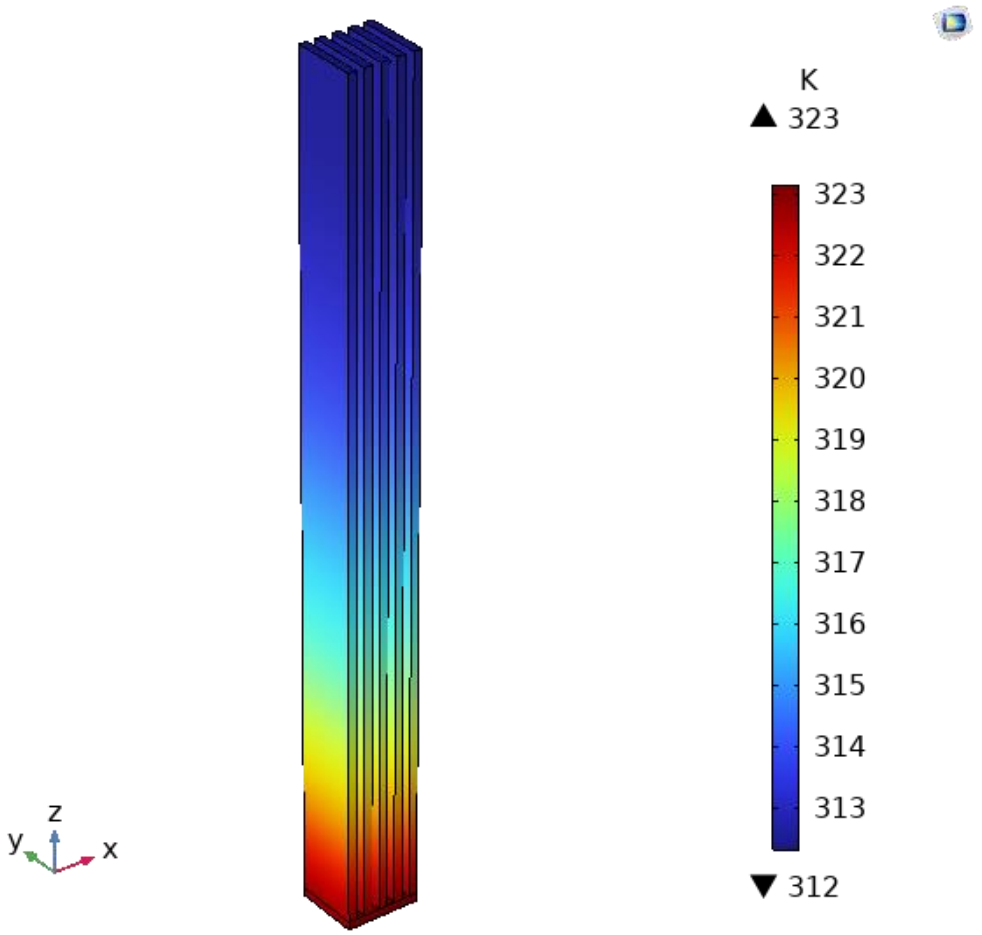
- Space dimension: 3D
- Physics model: Heat transfer in solids(ht)
- Study: Stationary

Geometry and Meshing – (Meshing category used: ‘Finer’)

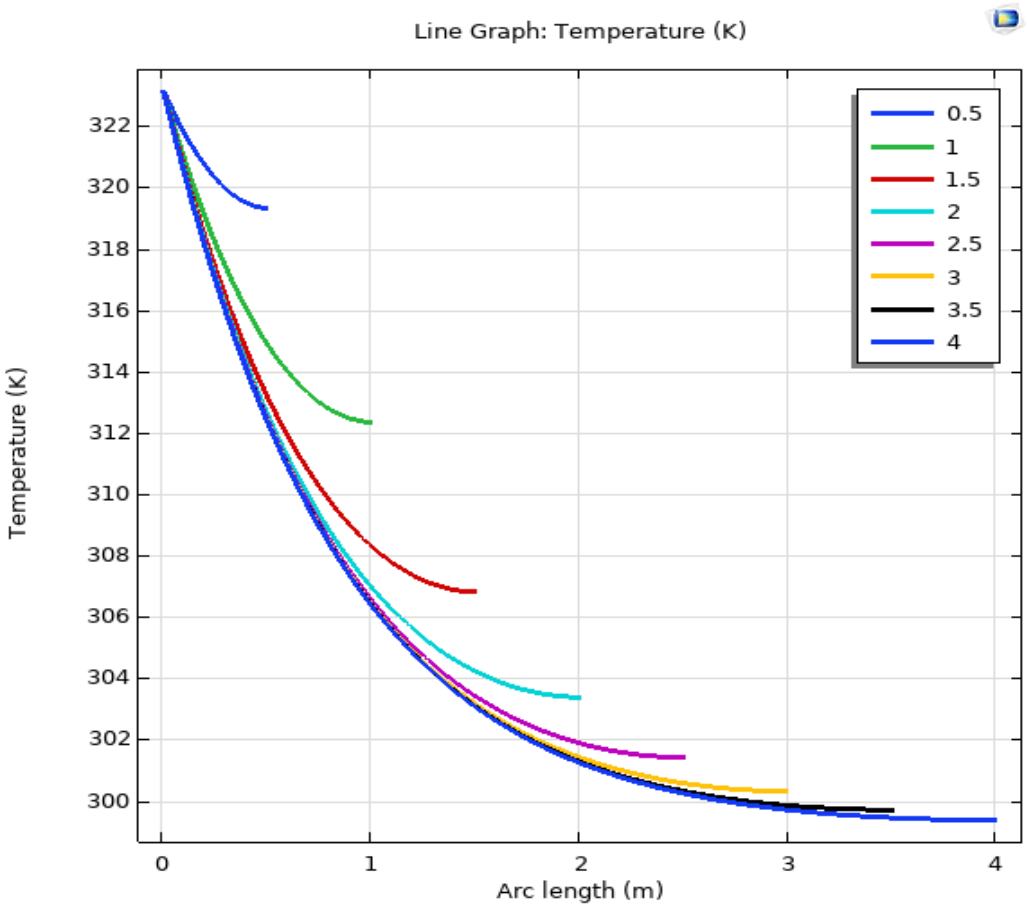




Temperature profile (3D Rainbow Plot) obtained for L = 1m –



Temperature profile (T vs x) for different fin lengths –



From the above Line Graph, we can see that the temperature comes within 99% of ambient temperature (298.85 K) after about 3 to 3.5 meters of fin length. Any extra length would be of little help. Hence, we can say that the **optimum length** in this case is **3 to 3.5 meters** respectively.

Note that this optimum length **does not match** the 0.7m optimised length we obtained in the **Simplified Model**. One possible reason for this can be the fact that the material used for this model (Copper) is different from the hypothetical material we used in the Simplified Model.

TASK 2

Situation: NH_3 to be absorbed from an air mixture counter-currently in a plate column with fresh water (no solute).

Important Points to consider:

- concept of **counter-current cascades** to be used
- **gas to liquid** solute transfer

Given data:

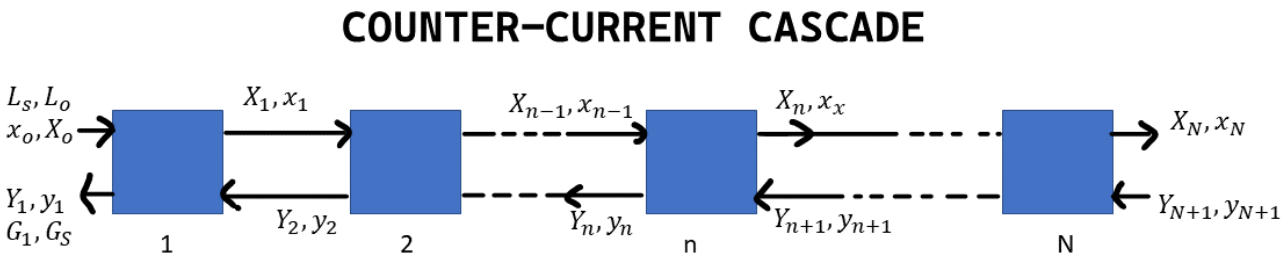
- initial NH_3 concentration
- final NH_3 concentration
- initially, the liquid stream does not contain any solute i.e. *fresh water*
- inlet water flow rate
- inlet gas mixture flow rate
- efficiency of each tray in the column = 70%
- molar masses of air, NH_3 and water are 29, 17 and 18 kg/mol

To report:

- operating line equation
- the number of *actual* plates required for the absorption column to achieve desired separation

RECAPITULATION

- initial NH_3 concentration = 10 mol%
- final NH_3 concentration = 1 mol%
- inlet water flow rate = 500 kg/s
- inlet gas mixture flow rate = 400 kg/s



Counter-current cascade setup with N stages.

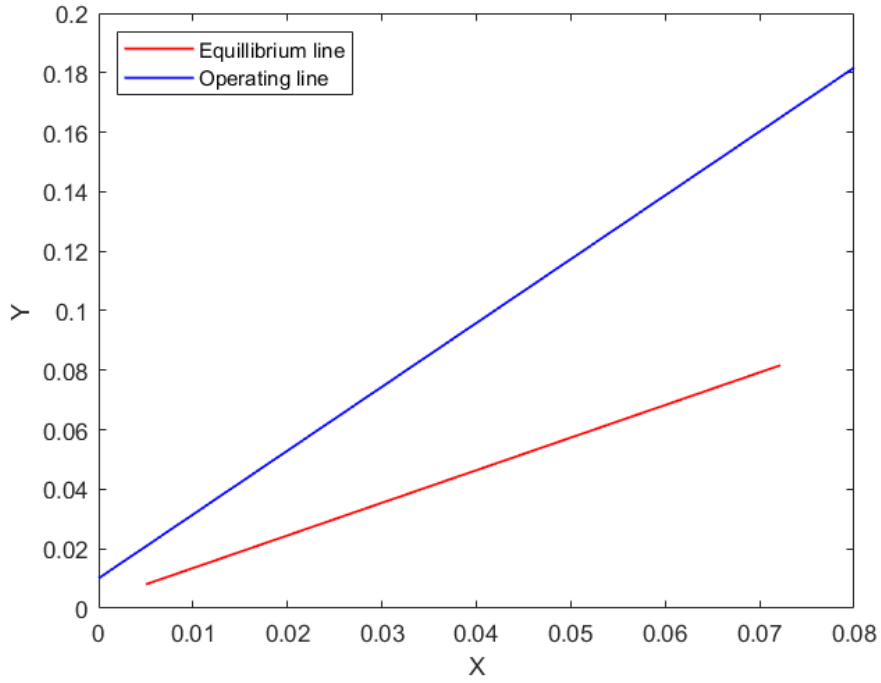
Applying material balance for solute at **nth stage** (/tray) -

$$\boldsymbol{Y_{n+1} - Y_n = \frac{L_s}{G_s} * (X_n - X_{n-1})}$$ where, 1 <= n <= N

Using the above equation and iterative process, we can obtain the operating line.

In the question, we are given – L_S, G_S, Y_1, Y_{N+1}, X_0

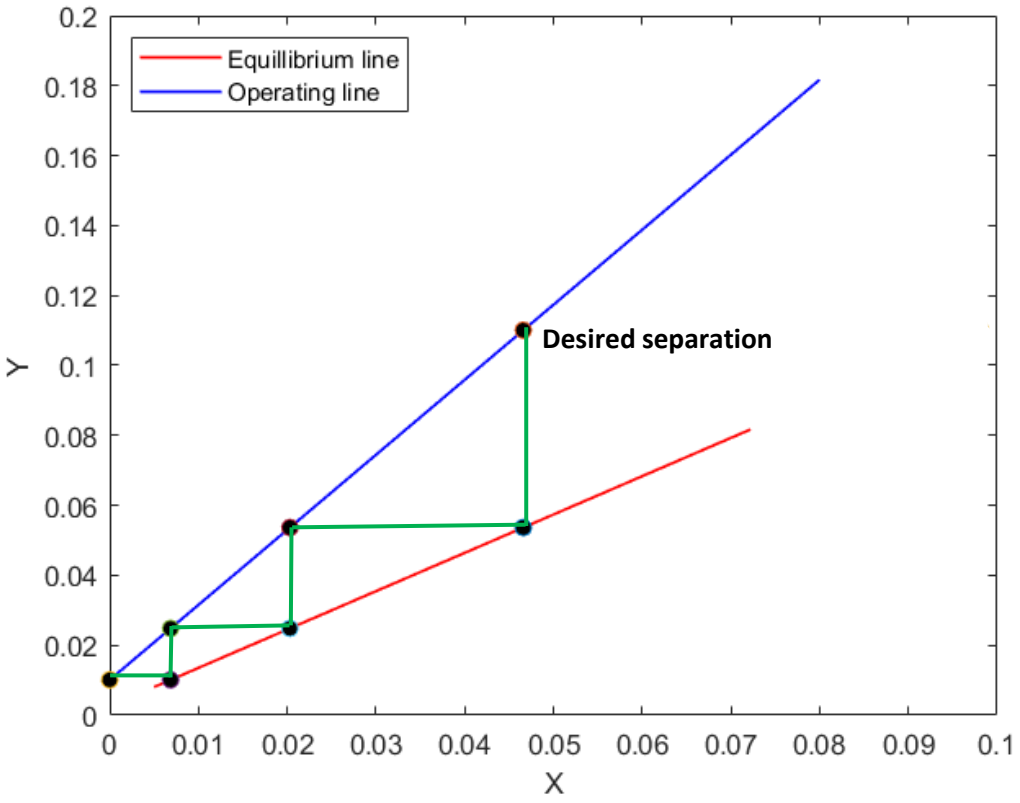
Based on the given data along with equilibrium line data, we obtained the following equations for the operating and the equilibrium line –



$$\boldsymbol{Equillibrium\ line \rightarrow Y = 1.096 * X + 0.002576}$$

$$\boldsymbol{Operating\ line \rightarrow Y = 2.14506 * X + 0.010101}$$

Using iterative process, we can calculate the number of trays required assuming a 100% efficiency for each tray as follows –



As we can see from the above graph,
trays required in order to achieve desired separation = 3.

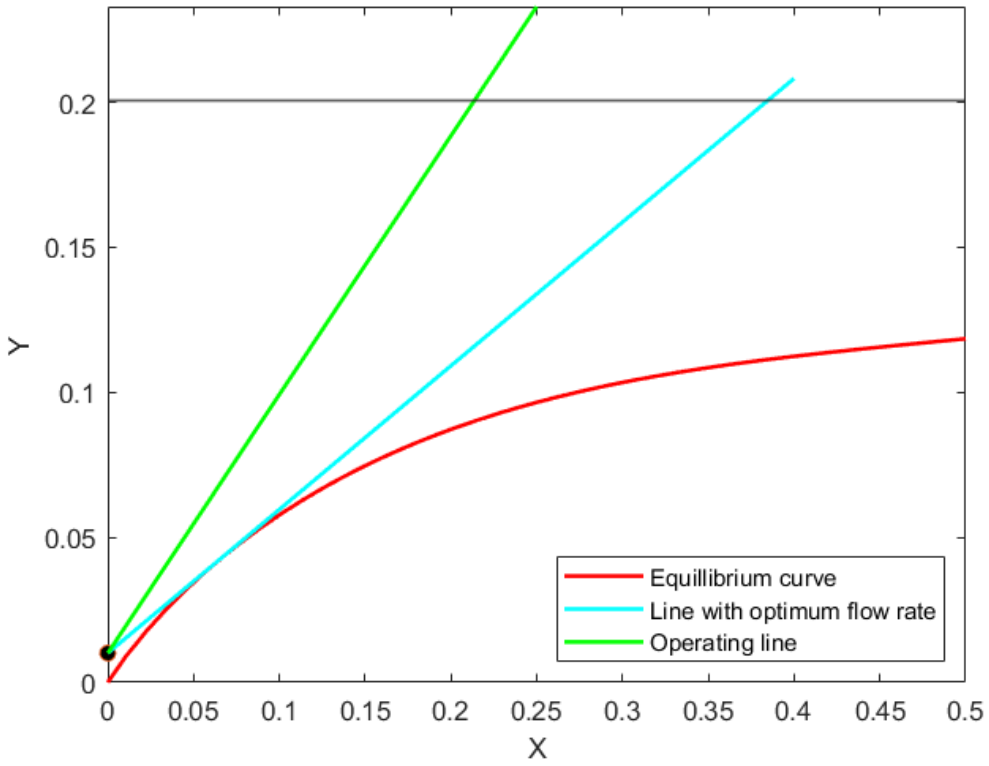
Therefore, **actual number** of trays required = 3/tray efficiency = 3/0.7 = **5** (ceil value).

OPTIMIZATION

Given data:

- initial NH_3 concentration = 16.7 mol%
- final NH_3 concentration = 1 mol%
- inlet water flow rate = L kg/s = 1.8 x L_{op}, where L_{op} is the optimum liquid flow rate
- inlet gas mixture flow rate = 500 kg/s

Using curve fitting on MATLAB for the equilibrium data given in the question and the inlet and outlet flow rates and concentrations of NH_3, we obtained the following curves –



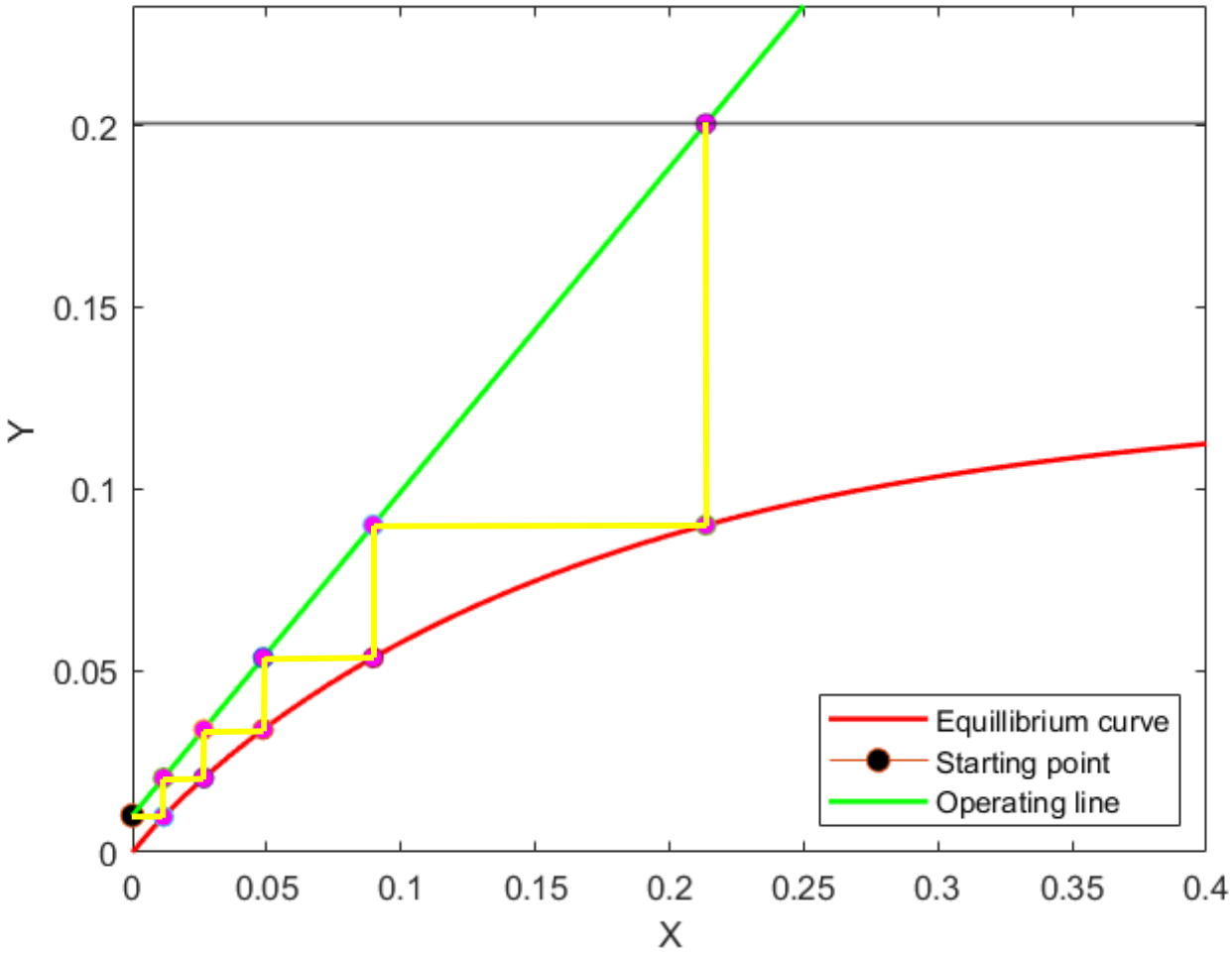
$$\boldsymbol{Equillibrium\ curve \rightarrow Y = -0.9996 - 1.499 * X^{1.5} + 0.9996 * e^{X}}$$

$$\boldsymbol{Operating\ line \rightarrow Y = 1.8 * 0.4953 * X + 0.010101}$$

Line with optimum flow rate is tangent to the equilibrium curve, we will not achieve the desired separation if the flow rate is below the optimum flow rate.

Slope of line with optimum flow rate = L_{op}/G_s
Slope of operating line = $L_s/G_s = 1.8L_{op}/G_s$

Now by using the iterative process (loop in MATLAB) we can calculate the number of trays required to achieve desired separation assuming ideal trays (100% efficiency).



From the graph, number of trays required = 5

Therefore, **actual number** of trays required = 5/tray efficiency = 5/0.7 = **8** (ceil value)

-END-