INDIAN INSTITUTE OF TECHNOLOGY KANPUR

DEPARTMENT OF CHEMICAL ENGINEERING

CHEMINEERS SOCIETY

SIMUTECH PROJECT

Submitted by

GROUP - ‘C’

PROJECT

On

Chemical Engineering Applications: Process, Modeling and Design

(ChEA: PMD)

Mentor: Sunny Kumar Bhagat

Group Members

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2.	Ayush Patel	200249
3.	Riya Saini	200810
4.	Ujwal Kumar	201061

WORK DISTRIBUTION

Task 1: Heat Transfer

- Ayush Patel:
  - ❖ Generated Temperature Profile w.r.t Fin length for different time length.
  - ❖ Reporting Optimized fin length.

- Akshat Bajaj:
  - ❖ Reported the structure drawn in COMSOL, meshing generated, and 3D rainbow plot of Temperature variation around fin's surface.
  - ❖ Temperature variation w.r.t x to check whether the fin was effective or not.
  - ❖ Cross check the length obtained as a result of a simplified model

Task 2: Absorption Column

- Riya Saini:
  - ❖ Analyzing the data given, and finding the equation of equilibrium line.
  - ❖ Reporting the operating line.

- Ujwal Kumar:
  - ❖ Calculating the number of trays with equilibrium line and operating line using python.

Task - 1

Part - 1

A rectangular fin cooler (0.09m X 0.01m X 0.08m) with a vertical fin installed at its center dimension being (0.01m X 1 m X 0.08m) is taken into consideration.
All related data is given in the problem itself.
Equation used -

$$dT/dt = c0*d^2T/dx^2 + c1*(T - T_{am})$$

Here, $c0 = -K*A\_cond/rho*A\_cond*c_p$, $c1 \; h*p/rho*A\_cond*c_p$

Now , the equation is being solved by using the central difference method and backward difference method.

To calculate the temperature at the last node we will use the backward difference method.

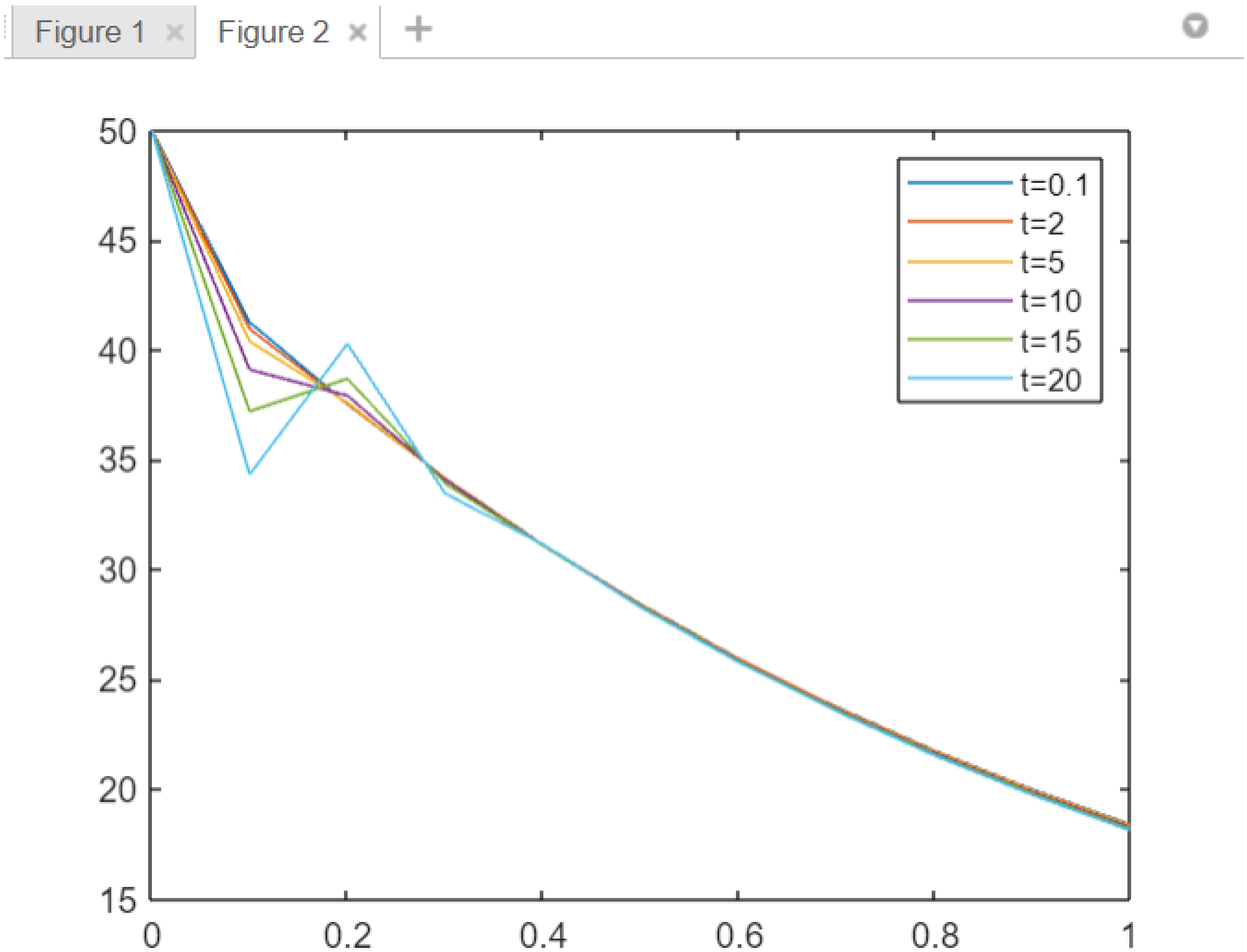
Here x denotes the node on which we are calculating the temperature, p denotes the time scale.

$$d^2T/dx^2 = T(x,p-1) - 2T(x,p) + T(x,p+1) / del\_x^2 ,$$

$$dT/dx = T(x,p+1) - T(x,p) / dt ,$$

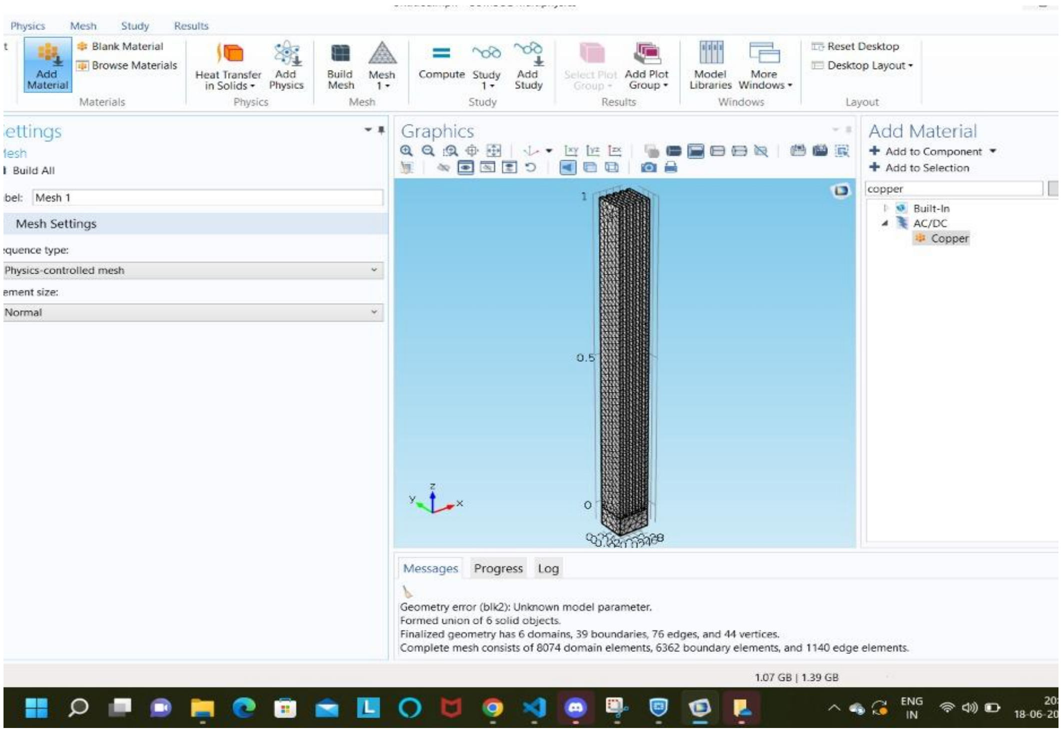
T(x,0) is given in the question which is = 50*exp(-x) + 1.6*x.

The result contains the temperature variation at particular time w.r.t x

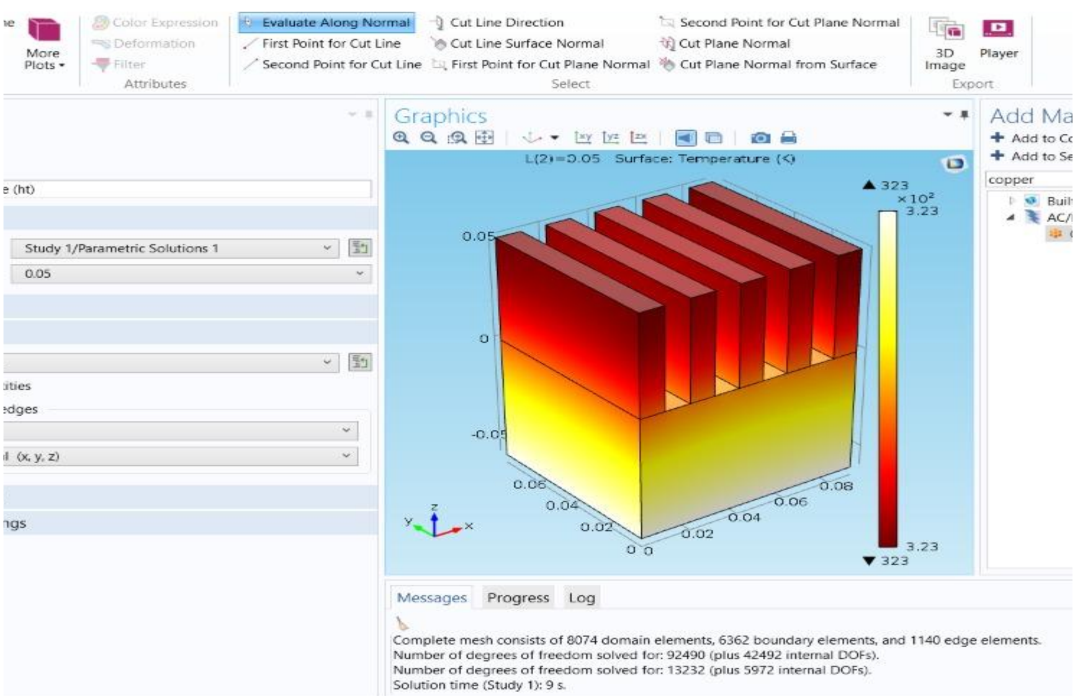


Optimized length is the length at which the fin tip temperature is approximately equal to ambient temperature.
The optimized length for this rectangular fin cooler is 0.6m.

Implementation Model

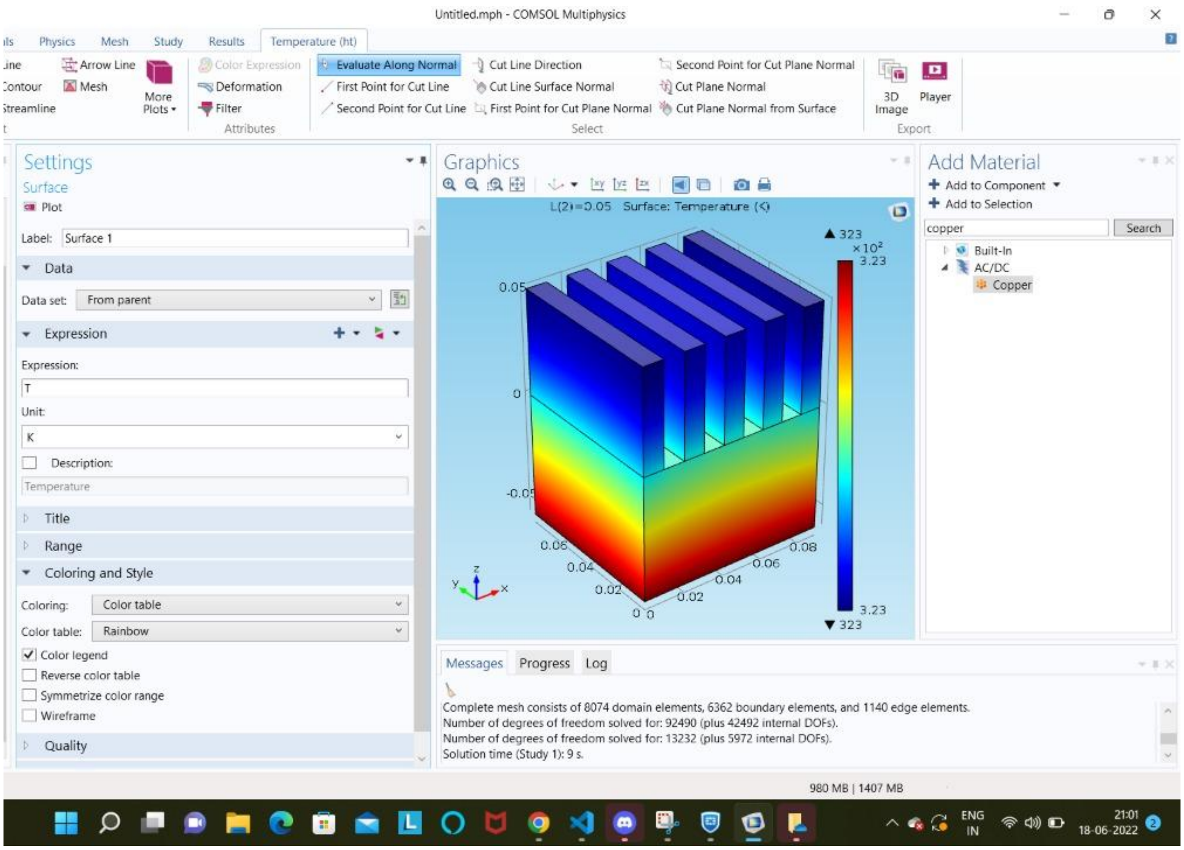


The above picture denotes the mesh analysis of a fin.



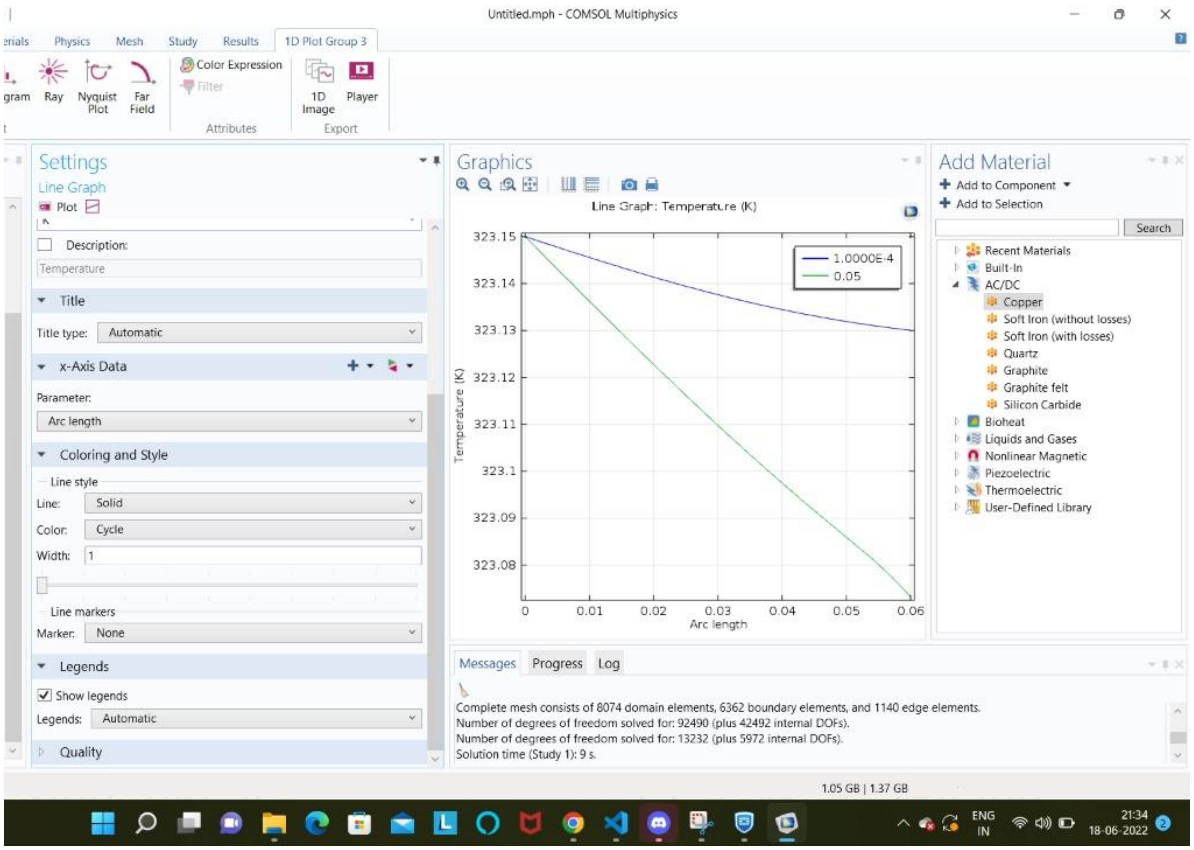
Temperature Profile

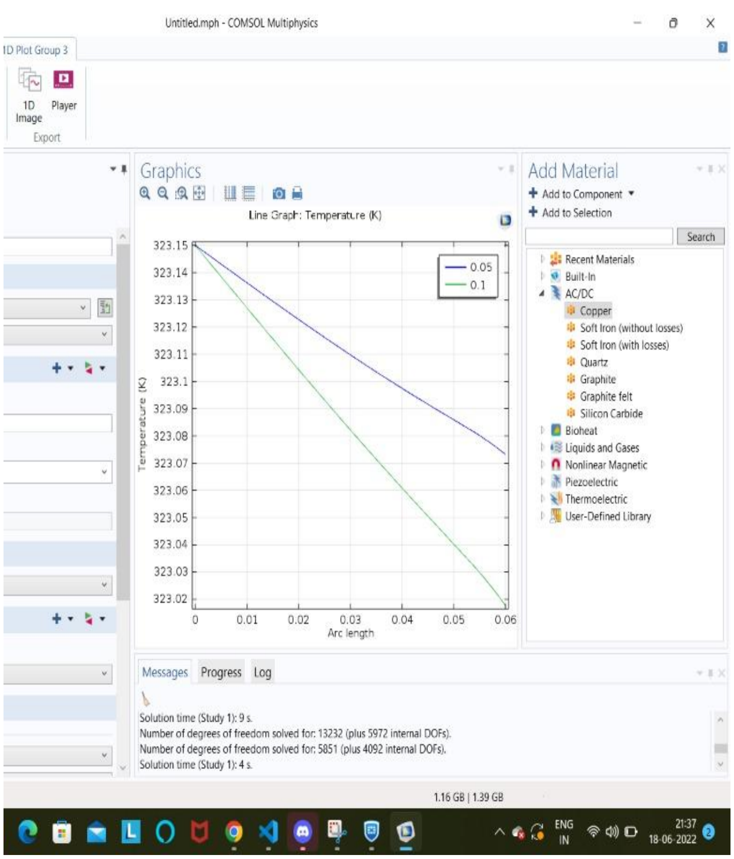
This is the temperature profile of the multi-fin system as shown above the base has a higher temperature and as we go up due to extended surface area as provided by the fin the temperature decreases and its variation can be seen clearly.



Temperature profile(3D Rainbow Plot) obtained shown above

Now the graph shown below is the temperature variation in fin at different length intervals by using parametric sweep (of h) from 0.0001 to 0.05 to 0.1 to 0.15 to 0.2.


Untitled.mph - COMSOL Multiphysics
Physics
Mesh
Study
Results
1D Plot Group 3
Ray
Nyquist Plot
Far Field
Color Expression
Filter
Attributes
1D Image
Player
Export
Settings
Line Graph
Plot
Description:
Temperature
Title
Title type: Automatic
x-Axis Data
Parameter:
Arc length
Coloring and Style
Line style
Line: Solid
Color: Cycle
Width: 1
Line markers
Marker: None
Legends
Show legends
Legends: Automatic
Quality
Graphics
Line Graph: Temperature (K)
1.0000E-4
0.05
Temperature (K)
Arc length
Add Material
Add to Component
Add to Selection
Search
Recent Materials
Built-In
AC/DC
Copper
Soft Iron (without losses)
Soft Iron (with losses)
Quartz
Graphite
Graphite felt
Silicon Carbide
Bioheat
Liquids and Gases
Nonlinear Magnetic
Piezoelectric
Thermoelectric
User-Defined Library
Messages
Progress
Log
Complete mesh consists of 8074 domain elements, 6362 boundary elements, and 1140 edge elements.
Number of degrees of freedom solved for: 92490 (plus 42492 internal DOFs).
Number of degrees of freedom solved for: 13232 (plus 5972 internal DOFs).
Solution time (Study 1): 9 s.
1.05 GB | 1.37 GB
ENG
IN
21:34
18-06-2022


Untitled.mph - COMSOL Multiphysics
1D Plot Group 3
1D Image
Player
Export
Graphics
Line Graph: Temperature (K)
0.05
0.1
Temperature (K)
Arc length
Add Material
Add to Component
Add to Selection
Search
Recent Materials
Built-In
AC/DC
Copper
Soft Iron (without losses)
Soft Iron (with losses)
Quartz
Graphite
Graphite felt
Silicon Carbide
Bioheat
Liquids and Gases
Nonlinear Magnetic
Piezoelectric
Thermoelectric
User-Defined Library
Messages
Progress
Log
Solution time (Study 1): 9 s.
Number of degrees of freedom solved for: 13232 (plus 5972 internal DOFs).
Number of degrees of freedom solved for: 5851 (plus 4092 internal DOFs).
Solution time (Study 1): 4 s.
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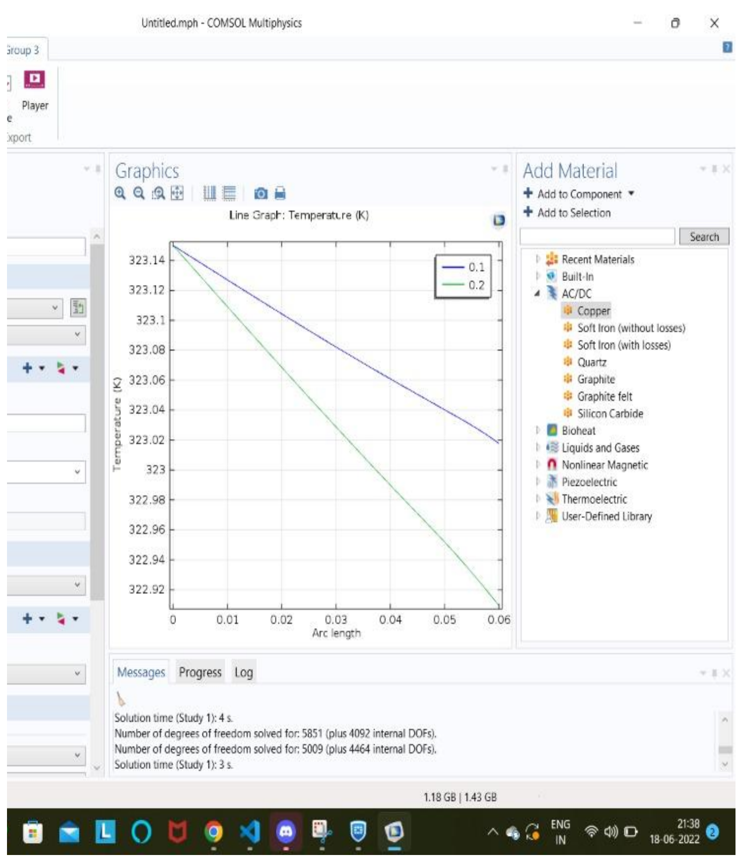
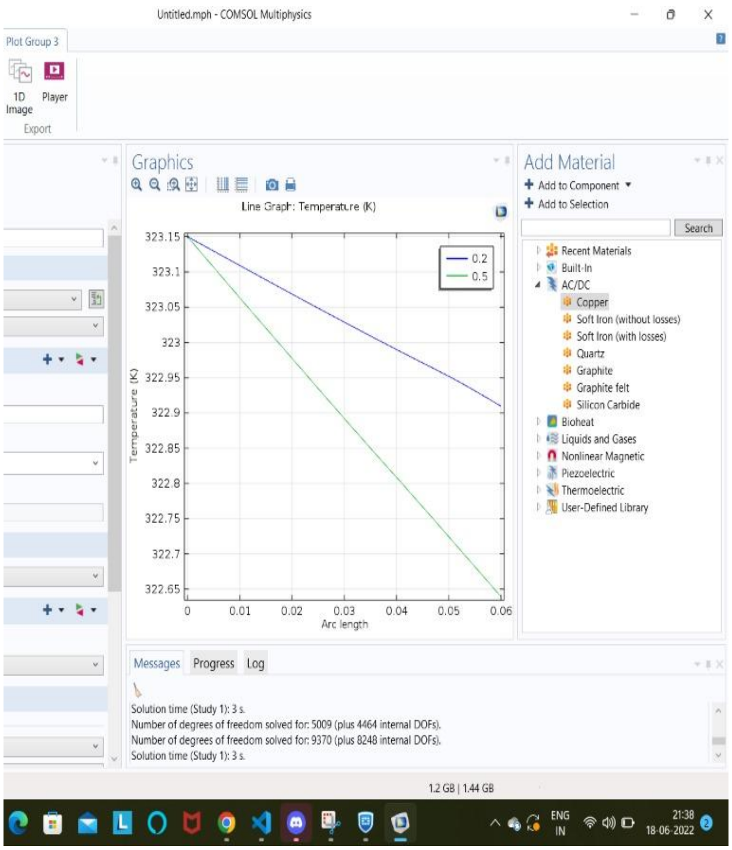
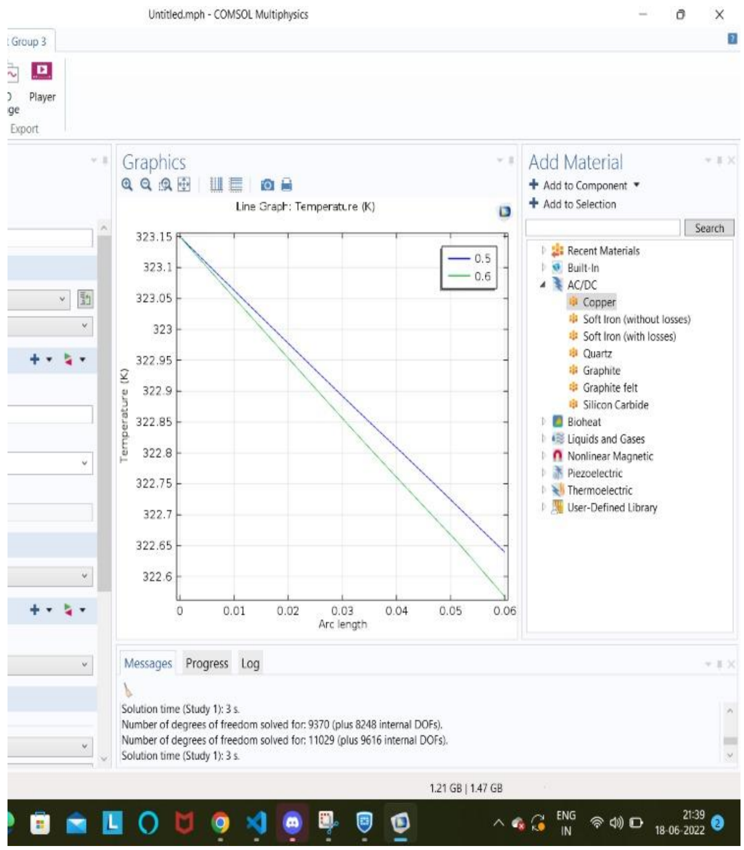
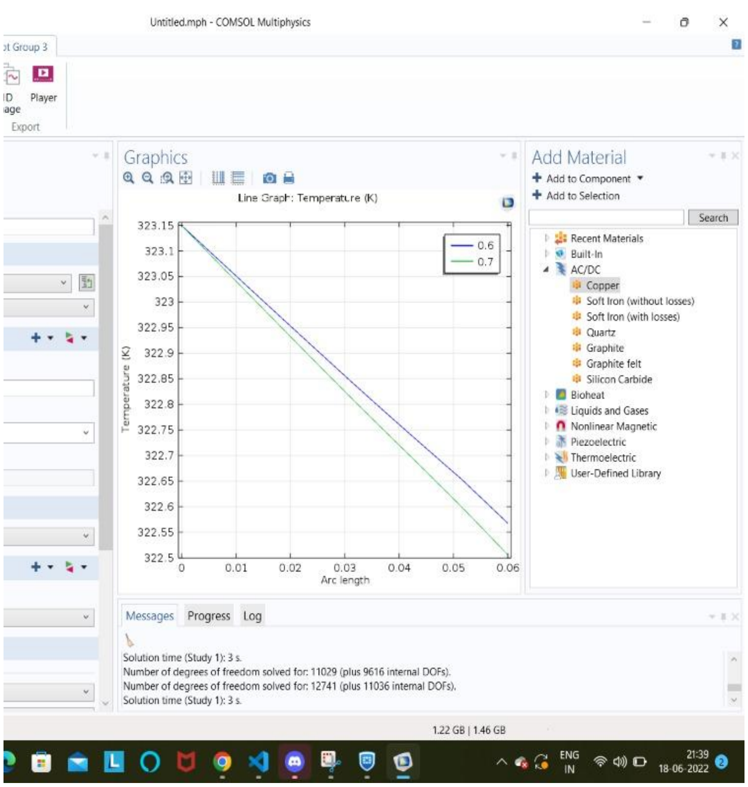
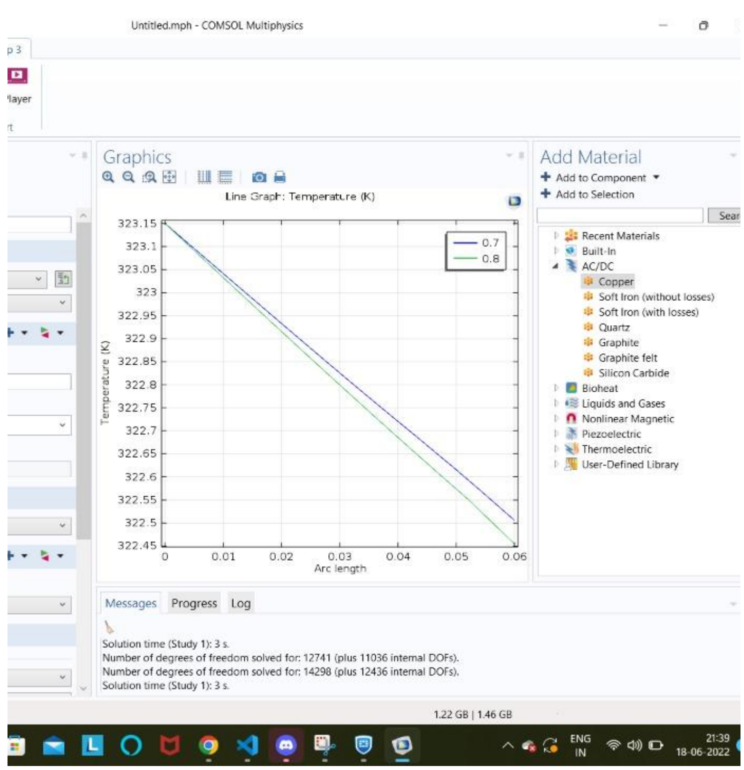
ENG
IN
21:37
18-06-2022


Untitled.mph - COMSOL Multiphysics
Player
Graphics
Line Graph: Temperature (K)
0.1
0.2
Temperature (K)
Arc length
Add Material
Add to Component
Add to Selection
Search
Recent Materials
Built-In
AC/DC
Copper
Soft Iron (without losses)
Soft Iron (with losses)
Quartz
Graphite
Graphite felt
Silicon Carbide
Bioheat
Liquids and Gases
Nonlinear Magnetic
Piezoelectric
Thermoelectric
User-Defined Library
Messages
Progress
Log
Solution time (Study 1): 4 s.
Number of degrees of freedom solved for: 5851 (plus 4092 internal DOFs).
Number of degrees of freedom solved for: 5009 (plus 4464 internal DOFs).
Solution time (Study 1): 3 s.
1.18 GB | 1.43 GB
ENG
IN
21:38
18-06-2022









As it can be seen the optimum fin length is greater than 1m.

Task 2

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

Inlet: Air+ NH_3 in the gas column and water in the liquid column.
Outlet: Air + NH_3 in the gas column and Water and NH_3 in the liquid column.

Molar Mass given for water, air, and ammonia are 18,29, and 17 respectively.
Inlet mass flow rates are 500 kg/s for water and 400 kg/s for gas.

$L1$ = input molar flow rate of liquid = 500/18 = 27.7778 kmol/s.
$G1$ = input molar flow rate of gas = 400/27.8 = 14.38848 kmol/s
$L1/G1$ = 1.93050

Ammonia concentration decreases from 10% to 1%. This means moles of ammonia decrease from 1.438848 to 0.1438848.

$L2$ = output molar flow rate of liquid = 27.7778-1.29496401 = 26.48283599 kmol/s
$G2$ = output molar flow rate of gas = 14.38848 - 1.29496401 = 13.0938489 kmol/s
$L2/G2$ = 2.022

$L1/G1$ and $L2/G2$ are approximately same.
Therefore **Ls/Gs is the average** of both which is 1.97625.

$Y(N+1)$(molar ratio at inlet) = moles of ammonia/moles of air = **0.11107**
$X(1)$(molar ratio at inlet) = moles of ammonia/moles of water = **0**

$Y(1)$ (molar ratio at outlet) = moles of ammonia/moles of air = **0.01111**

From operating line equation:

Y(N+1) - Y1 = (Ls/Gs)(X(N) - X(1))

Putting values we get,

X(N) = 0.050599

Now we have two endpoints of absorption column

P(0,0.01111)

Q(0.050599, 0.11107)

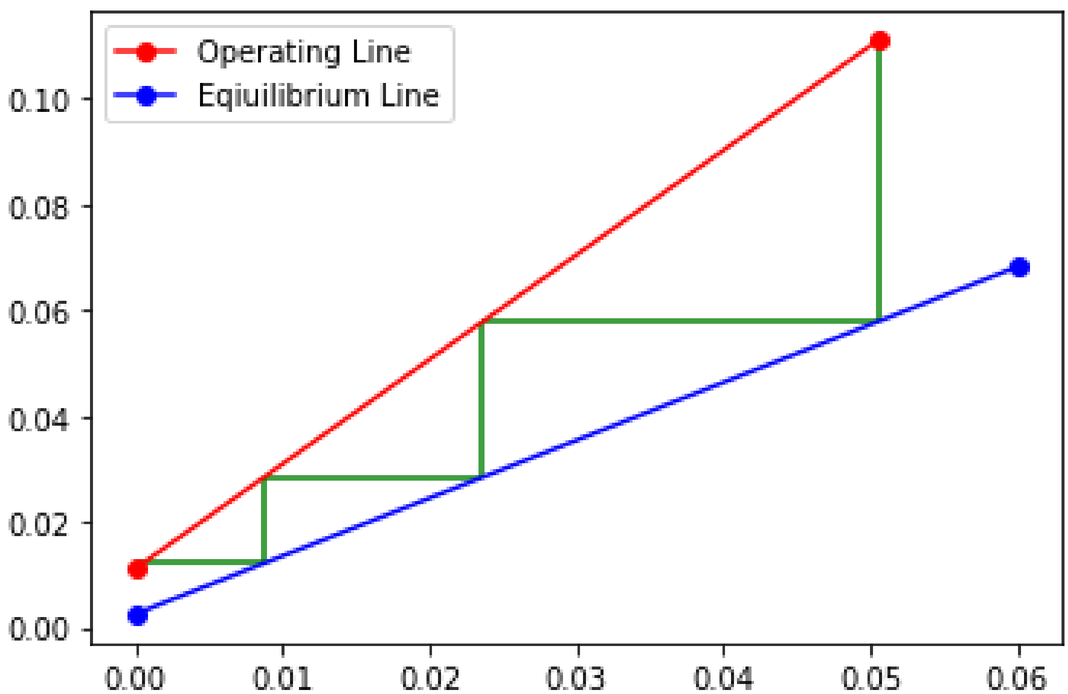
And operating line is **Y = 1.97625X + 0.01111**

Now by analysing data and by linear regression we found equilibrium equation

Y = 1.09559X + 0.00257.

For calculating a number of trays, the algorithm obtained is:

A. Take the ordinate of point P and draw a horizontal line to meet the equilibrium line, and calculate respective abscissa at that ordinate using the equation.
B. Now take calculate abscissa and draw a vertical line to meet the operating line that makes one tray.
C. Calculate steps A and B till the vertical line meets the ordinate of Q.



Seeing the graph, we see 3 trays.
But in the question, it is given that tray is **70% efficient**
Number of real trays = ideal tray/stage efficiency = **3/0.7 = 4.28 = 5 trays.**

Optimization:

Now we have an equilibrium line in form of a curve,
Put three data points given in the curve to get 3 different equation in A, B, C and solve it using the method taught in ESO208 LU decomposition.
We get A = 0.997398, B = 1.493892 ,C = 0.997398
Equilibrium Equation:
$Y = -0.99738 - 1.493892*x^{1.5} + 0.997398*e^{x}$

Mass flow rate for **gas** is = **500 kg/s** (given)
Molar flow rate will be = 500/27.8 = **17.9856**

Ammonia concentrations decreases from 16.7% to 1%.
Moles of ammonia in gas inlet = 3.00352
Y(N+1) = 0.200799
X(1) = 0
Y(1) = 0.0120048

Right now we have one point for operating line i.e. **(0,0.0120048)**
To know the Molar flow rate for liquid, we need to find optimum flow rate
For that we need to find the equation passing through P and touching the curve.
The algorithm used:

1.) Calculate the slope of equilibrium line
2.) Let's say it passes through the point (x0, y0)
3.) Now get the equation of a line in form of x0 and solve for x0.
4.)Use ESO208 method newton raphson to calculate x0.

We get the value of x = 0.06885

Using this calculated slope Ls/Gs

Optimum flow rate comes out to be = 128.586 kg/s

Now our flow rate for the question is 1.8*128.586 = 231.456 kg/s

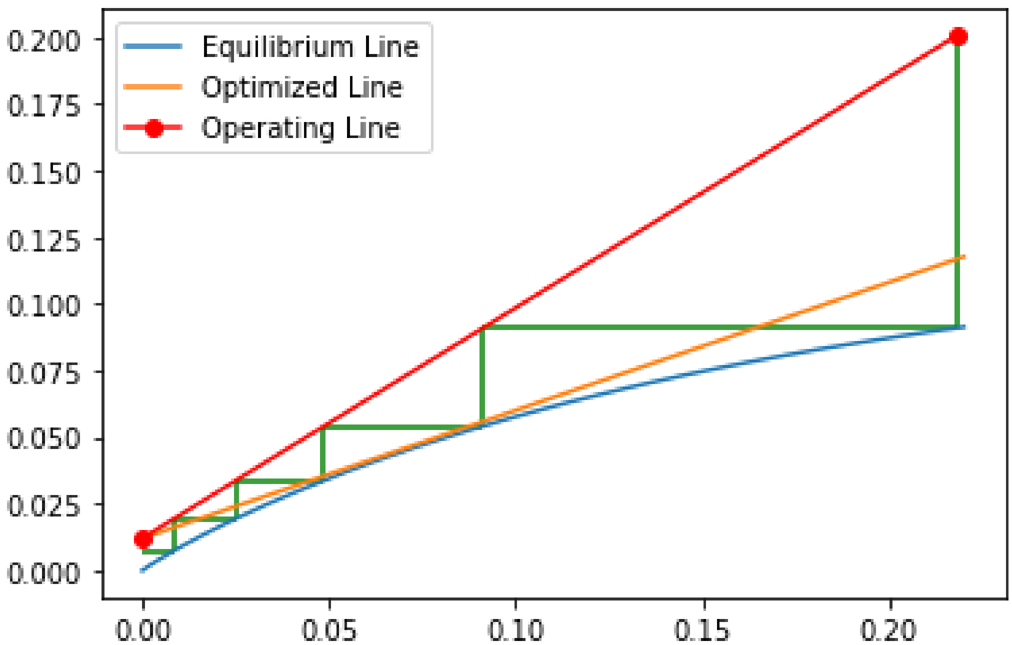
Molar flow rate is = 12.85867

Now doing the same thing did for subpart 1

We get **P(0,0.0120048) and Q (0.21799,0.2004799)**

And operating line is **Y = 0.86460*X + 0.0120048**

Using same algorithm to calculate number of trays,



Seeing graph we have **5 trays**

For this also we have 70% efficiency

Number of real trays = **ideal tray/ efficiency** = 5/0.7 = 7.14 = **8 trays**