Lab Session 3

Submitted By: Priyanshu Maurya

Roll No.: 220827

TA: Praful Mane

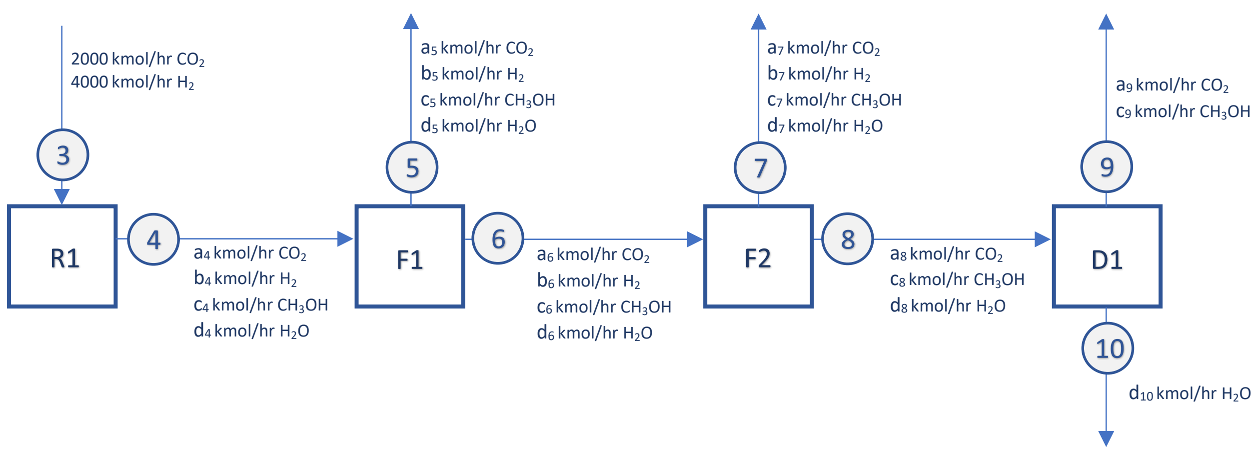
AIM

The goal of the laboratory session is to determine the total molar flow rates of all the streams and make a contour plot illustrating the variation of CH_3OH production cost as a function of CO_2 and H_2 prices.

METHOD

Approach 1: We first assign variables to different molar rates at each process as shown below,

a3 = 2000 kmol/hr
b3 = 4000 kmol/hr



Approach 2: Using appropriate mass and energy balances, we can form equations as follows:

Equations at reactor flask:

$a_4 = 0.6675*a_3$
$b_4 = b3 – 0.9975*a_3$
$c_4 = 0.3325*a_3$
$d_4 = 0.3325*a_3$

Equations at flash drum 1:

$a_5 = 0.972*a_4$
$b_5 = 0.9927*b_4$
$c_5 = 0.0235*c_4$
$a_6 = a_4 – a_5$
$b_6 = b_4 – b_5$
$c_6 = c_4 – c_5$
$d_6 = d_4 – d_5$

Equations at flash drum 2:

$a_7 = 30.89* a_8$

$b_7 = b_6$

$c_7 = 0.0125*c_8$

$d_7 = 0.00265*d_8$

$a_8 = 0.031*a_6$

$c_8 = 0.987*c_6$

$d_8 = 0.997*d_6$

Equations at distillation column:

$a_9 = a_8$

$c_9 = c_8$

$d_{10} = d_8$

Approach 3: We have the following matrix equation. Using MATLAB function linsolve, we will solve for variables:

$$\begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-0.972 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & -30.89 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -0.031 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -0.972 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.024 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -0.013 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.987 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -0.003 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.997 & 0 & 1
\end{bmatrix}
\begin{bmatrix} a_4 \\ a_5 \\ a_6 \\ a_7 \\ a_8 \\ b_4 \\ b_5 \\ b_6 \\ b_7 \\ c_4 \\ c_5 \\ c_6 \\ c_7 \\ c_8 \\ d_4 \\ d_6 \\ d_7 \\ d_8 \end{bmatrix}
=
\begin{bmatrix} 0.6675*a_3 \\ 0 \\ 0 \\ 0 \\ 0 \\ b_3-0.9975*a_3 \\ 0 \\ 0 \\ 0 \\ 0.3325*a_3 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0.3325*a_3 \\ -3.103 \\ 0 \\ 0 \end{bmatrix}$$

RESULTS and ANALYSIS

After solving using linsolve in MATLAB we get:

Total molar flow rates for:

$n_4 = 4670$ kmol/hr

$n_5 = 3306.70$ kmol/hr

$n_6 = 1363.27$ kmol/hr

$n_7 = 60.58$ kmol/hr

$n_8 = 1302.66$ kmol/hr

$n_9 = 642.52$ kmol/hr

$n_{10} = 660.14$ kmol/hr

For stream 4:

$a_4 = 1335$ kmol/hr CO_2

$b_4 = 2005$ kmol/hr H_2

$c_4 = 665$ kmol/hr CH_3OH

$d_4 = 665$ kmol/hr H_2O

For stream 5:

$a_5 = 1297.6$ kmol/hr CO_2

$b_5 = 1990.4$ kmol/hr H_2

c_5 = 15.6 kmol/hr CH_3OH
d_5 = 3.103 kmol/hr H_2O

For stream 6:

a_5 = 37.38 kmol/hr CO_2
b_5 = 14.63 kmol/hr H_2
c_5 = 649.37 kmol/hr CH_3OH
d_5 = 661.89 kmol/hr H_2O

For stream 7:

a_5 = 36.20 kmol/hr CO_2
b_5 = 14.63 kmol/hr H_2
c_5 = 8.01 kmol/hr CH_3OH
d_5 = 1.74 kmol/hr H_2O

For stream 8:

a_5 = 1.17 kmol/hr CO_2
c_5 = 641.35 kmol/hr CH_3OH
d_5 = 660.14 kmol/hr H_2O

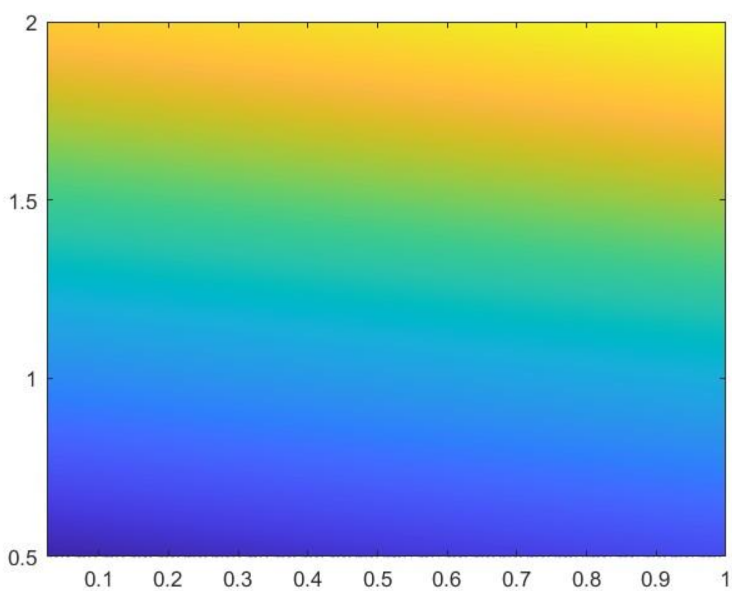
For stream 9:

a_5 = 1.17 kmol/hr CO_2
c_5 = 641.35 kmol/hr CH_3OH

For stream 10:

d_5 = 660.14 kmol/hr H_2O

The contour plot illustrating the variation of CH_3OH production cost as a function of CO_2 and H_2 prices is shown below:



CONCLUSION

We got the molar flow rate for all the processes. Then we calculated the variation of cost of production of CH_3OH by varying the prices of CO_2 and H_2 in the feed. Using this data, we plotted this on a contour graph.

APPENDIX

The MATLAB code to solve the problem is as follows:

```
CO2_3 =2000;
H2_3 = 4000;
% Using equations, we get following matrix
A= [1      0 0      0 0      0     0  0 0  0     0  0     0  0     0 0 0 0;
    -0.972 1 0      0 0      0     0  0 0  0     0  0     0  0     0 0 0 0;
    -1     1 1      0 0      0     0  0 0  0     0  0     0  0     0 0 0 0;
    0      0 0      1 -30.89 0     0  0 0  0     0  0     0  0     0 0 0 0;
    0      0 -0.031 0 1      0     0  0 0  0     0  0     0  0     0 0 0 0;
    0      0 0      0 0      1     0  0 0  0     0  0     0  0     0 0 0 0;
    0      0 0      0 0     -0.972 1  0 0  0     0  0     0  0     0 0 0 0;
    0      0 0      0 0     -1     1  1 0  0     0  0     0  0     0 0 0 0;
    0      0 0      0 0      0     0 -1 1  0     0  0     0  0     0 0 0 0;
    0      0 0      0 0      0     0  0 0  1     0  0     0  0     0 0 0 0;
    0      0 0      0 0      0     0  0 0 -0.024 1  0     0  0     0 0 0 0;
    0      0 0      0 0      0     0  0 0 -1     1  1     0  0     0 0 0 0;
    0      0 0      0 0      0     0  0 0  0     0  0     1 -0.013 0 0 0 0;
    0      0 0      0 0      0     0  0 0  0     0 -0.987 0  1     0 0 0 0;
    0      0 0      0 0      0     0  0 0  0     0  0     0  0     1 0 0 0;
    0      0 0      0 0      0     0  0 0  0     0  0     0  0    -1 1 0 0;
    0      0 0      0 0      0     0  0 0  0     0  0     0  0     0 0 1 -0.003;
    0      0 0      0 0      0     0  0 0  0     0  0     0  0     0 -0.997 0 1];

b= [0.6675*CO2_3; 0; 0; 0; 0; H2_3-0.9975*CO2_3; 0; 0; 0; 0.3325*CO2_3; 0; 0; 0; 0; 0.3325*CO2_3;
-3.103; 0; 0];
x = linsolve(A, b);

% flow rates of streams 4, 5, 6, 7, 8, 9 and 10
n4=x(1)+x(6)+x(10)+x(15);
n5=x(2)+x(7)+x(11)+3.103;
n6=x(3)+x(8)+x(12)+x(16);
n7=x(4)+x(9)+x(13)+x(17);
n8=x(5)+x(14)+x(18);
n9=x(5)+x(14);
n10=x(18);

% C_op calculation
C_ele = (9.7+21.5)*72*3600;
C_steam = (0.28+0.8+15.7)*1000*3600*2.5*(10^-6);
C_cool = (12+20.9+22.6+15.4)*1000*3600*2.12*(10^-7);

% graph
cost_CO2 = linspace(0.025,1,100);
cost_H2 = linspace(0.5,2,100);
P_CH3OH = (7884*(x(14)*32/1000));
phi = 0.1;
F3 = CO2_3*44 + H2_3*2;
C_cap = 14694200 + 29418000 + (1.53*(10^7)*((F3/54000)^0.65)) + 269600 + 171300 + 168100 + 63000 +
1507900;

for i=1:100
    for j=1:100
        C_op(i,j) = (C_ele + C_steam + C_cool + (2000*44)*cost_CO2(i) + (4000*2)*cost_H2(j))*7884;
        TAC(i,j) = phi*C_cap + C_op(i,j);
        C_methanol(i,j) = TAC(i,j)/P_CH3OH;
    end
end
contour(cost_CO2, cost_H2, C_methanol,1000);
```