Purification of Methanol

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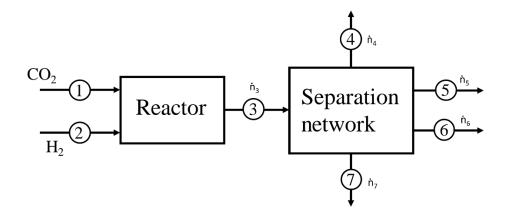
AIM

The goal of the laboratory session is to:

- 1) Determine the total molar flow rate of all the streams and the mole fractions of streams 4a and 5a.
- 2) Make a plot of the total capital cost of separation equipment as a function of product flow rate (stream 7).

METHOD

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



Approach 2: To find degree of freedom:

Number of variables = 4

Number of mass balance equations = 4

Therefore, degree of freedom = (Number of variables) – (Number of mass balance equations)

= 0

Approach 3: Using appropriate mass and energy balances, we can form equations as follows:

$$n_7 = 893.263 \text{ kmol/hr}$$

$$0.176(n_3) - 0.243(n_4) - 0.744(n_5) = 0.002(n_7)$$

$$0.53(n_3) - 0.752(n_4) - 0.027(n_5) = 0$$

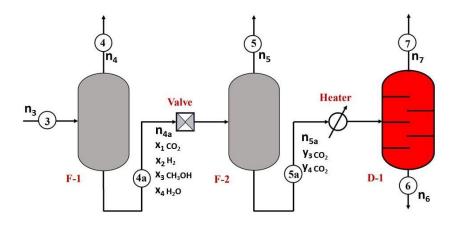
$$0.147(n_3) - 0.004(n_4) - 0.188(n_5) = 0.987(n_7)$$

 $0.147(n_3) - 0.001(n_4) - 0.041(n_5) - n_6 = 0.011(n_7)$

Approach 4: We have the following matrix equation. Using MATLAB function linsolve, we will solve for n_3 , n_4 , n_5 , & n_6

$$\begin{bmatrix} 0.176 & -0.243 & -0.744 & 0 \\ 0.530 & -0.752 & -0.027 & 0 \\ 0.147 & -0.004 & -0.188 & 0 \\ 0.147 & -0.001 & -0.041 & -1 \end{bmatrix} \begin{bmatrix} \mathbf{n_3} \\ \mathbf{n_4} \\ \mathbf{n_5} \\ \mathbf{n_6} \end{bmatrix} = \begin{bmatrix} 0.002(\mathbf{n_7}) \\ 0 \\ 0.987(\mathbf{n_7}) \\ 0.011(\mathbf{n_7}) \end{bmatrix}$$

Approach 5: Assigning variables to mole fractions of streams 4a and 4b:



Approach 6: After getting $n_3 \ n_4 \ n_5 \ n_6$, solving for n_{4a} and n_{5a} :

$$n_3 = n_4 + n_{4a}$$

$$n_{5a} = n_7 + n_6$$

Approach 7: Solving for x1, x2, x3, x4, y3, and y4 using equations below in MATLAB:

$$x_1 = ((0.176* \ \textbf{n}_3) - (0.243* \ \textbf{n}_4))/ \ \textbf{n}_{4a};$$

$$x_2 = ((0.53* N_3) - (0.752* N_4))/ N_{4a};$$

$$x_3 = (0.147* n_3)/ n_{4a};$$

$$x_4 = (0.147* n_3)/ n_{4a};$$

$$y_3 = (0.987* n_7)/ n_{5a}$$
;

$$y_4 = n_6 / n_{5a}$$
;

RESULTS AND ANALYSIS

After solving using linsolve in MATLAB we get:

 $n_3 = 6163.5 \text{ kmol/hr}$

 $n_4 = 4342.6 \text{ kmol/hr}$

 $n_5 = 37.3 \text{ kmol/hr}$

 $n_6 = 890.3 \text{ kmol/hr}$

 n_{4a} = 1820.9 kmol/hr

 $n_{5a} = 1783.6 \text{ kmol/hr}$

Mole fractions of stream 4a:

mole fraction of $CO_2 = 0.0162$

mole fraction of $H_2 = 0.00055$

mole fraction of CH₃OH = 0.4976

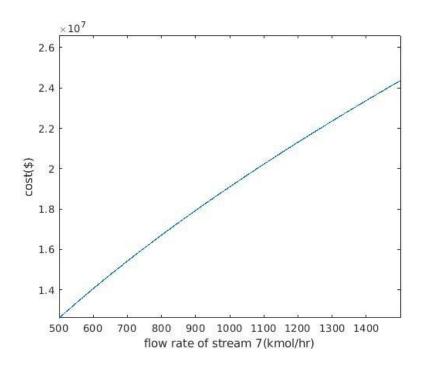
mole fraction of $H_2O = 0.4976$

Mole fractions of stream 5a:

mole fraction of CH₃OH = 0.4943

mole fraction of $H_2O = 0.4992$

The plot of the total capital cost of separation equipment as a function of product flow rate (stream 7) is shown below:



CONCLUSION

We got the molar flow rate for all the processes. And we also verified the value obtained from linsolve, using Gauss Elimination.

APPENDIX

The MATLAB code to solve the problem is as follows:

```
n7= 893.263;

cf1= [];

cf2= [];

cd1= [];

cost = [];

x= [];

A=[0.176 -0.243 -0.744 0;

0.53 -0.752 -0.027 0;

0.147 -0.004 -0.188 0;

0.147 -0.001 -0.041 -1];

b = [0.002*n7;

0;

0.987*n7;

0.011*n7];
```

```
% using linsolve function to solve matrix equation
n= double(linsolve(A, b));
n4a = n(1)-n(2);
n5a = n(4) + n7;
x1 = ((0.176*n(1)) - (0.243*n(2)))/n4a;
x2 = ((0.53*n(1)) - (0.752*n(2)))/n4a;
x3 = (0.147*n(1))/n4a;
x4 = (0.147*n(1))/n4a;
y3 = (0.987*n7)/n5a;
y4 = n(4)/n5a;
% plotting capital cost as function of inlet flow rate
for i = 500:1500
  m = i-499;
  f3 = i*(0.987/0.147);
  f4a = f3*(0.147/0.4976);
  f5a = i*(0.987/0.4943);
  cf1(m) = 182100*((f3/n(1))^{(0.6)});
  cf2(m)= 171200*((f4a/n(2))^(0.6));
  cd1(m)= 1725400*((f5a/n(3))^(0.6));
  cost(m) = cf1(m)+cf2(m)+cd1(m);
  x(m) = i;
end
plot(x, cost)
```