Lab Session 8

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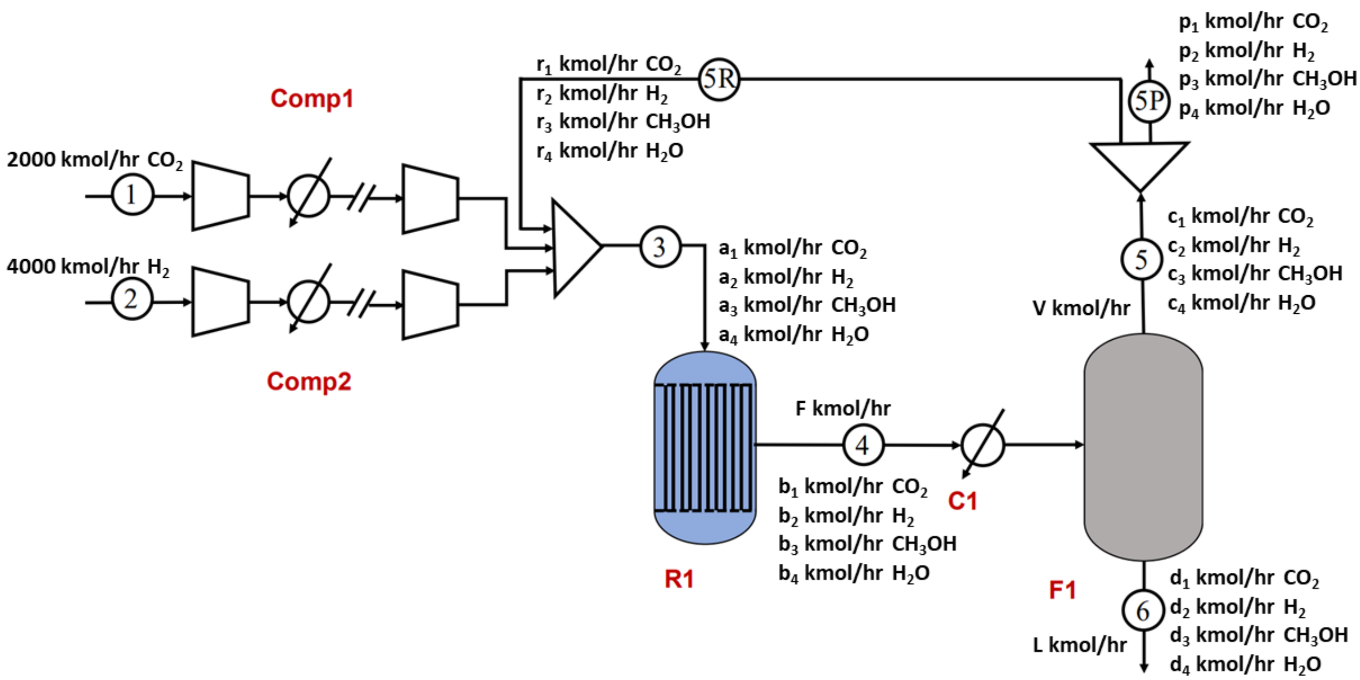
AIM

The aim of this session is to implement the sequential modular approach to find the molar flow rates of all the streams.

METHOD

Approach 1: It is given that the molar flow rate of CO_2 is 2000 kmol/hr. So, we can calculate molar flow rate of H_2 in stream 2 as 4000 kmol/hr.

Approach 2: Let molar flow rates of stream 3 be a_1, a_2, a_3 and a_4 for CO_2, H_2, H_2O and CH_3OH respectively. Similarly, b_1, b_2, b_3 and b_4 for stream 4; c_1, c_2, c_3 and c_4 for stream 5; d_1, d_2, d_3 and d_4 for stream 6. Also let F be total molar flow rate of stream 4, V be total molar flow rate of stream 5 and L be total molar flow rate of stream 6.



Approach 3: Using the values of coefficients of Antoine equation, we will calculate the value of K for CO_2, H_2, H_2O and CH_3OH using the below formula:

$$K = \frac{e^{\left(A - \frac{B}{T}\right)}}{P}$$

Approach 4: Using the values of K and initial guess as 1000 kmol/hr for each component of recycle stream, the value of Ψ can be calculated using the following equation,

$$0 = \sum_{i=0}^{4} \frac{Z_i * (1-K_i)}{1+\Psi*(K_i-1)}$$

Approach 5: The following equations are obtained because of molar flow rate balances on the reactor and the flash drum.

$a_1=r_1+2000$
$a_2=r_2+4000$
$a_3=r_3$
$a_4=r_4$
$b_1=0.7*a_1$
$b_2=a2-0.9*a_1$
$b_3=0.3*a_1+a_3$
$b_4=0.3*a_1+a_4$

Total molar flow rate equations are,

$F=b_1+b_2+b_3+b_4$
$V= \Psi*F$
$L=F-V$

Let z_1, z_2, z_3 and z_4 be mole fraction of CO_2, H_2, H_2O and CH_3OH respectively at stream 4.
Similarly, x_1, x_2, x_3 and x_4 be mole fractions of stream 6; y_1, y_2, y_3 and y_4 be mole fraction of stream 5.
Where,

$z_1=\frac{b_1}{F}$
$z_2=\frac{b_2}{F}$
$z_3=\frac{b_3}{F}$
$z_4=\frac{b_4}{F}$
$x_1=\frac{Z_1}{1+\Psi*(K_1-1)}$
$x_2=\frac{Z_2}{1+\Psi*(K_2-1)}$
$x_3=\frac{Z_3}{1+\Psi*(K_3-1)}$
$x_4=\frac{Z_4}{1+\Psi*(K_4-1)}$

Therefore, molar flow rate of stream 5 and 6 can be equated as,

$c_1=x_1*K_1*V$
$c_2=x_2*K_2*V$
$c_3=x_3*K_3*V$
$c_4=x_4*K_4*V$
$d_1=x_1*L$
$d_2=x_2*L$
$d_3=x_3*L$
$d_4=x_4*L$

Approach 6: Further, using the value of c_1, c_2, c_3 and c_4, we calculate the new value of r_1, r_2, r_3 and r_4.

$r_1=0.95*c_1$
$r_2=0.95*c_2$

$r_3=0.95*c_3$

$r_4=0.95*c_4$

Approach 7: We will iterate through until the difference between the previous value and the current value recycle stream is greater than tolerance. This way we can get molar flow rate of each stream by guessing the recycle stream and iterating it.

RESULTS AND ANALYSIS

The following table lists the molar flow rates of each stream in kmol/hr,

Components	Stream 3	Stream 4	Stream 5	Stream 5R	Stream 5P	Stream 6
CO_2	4058.82	2841.17	2167.18	2058.82	108.35	673.99
H_2	10352	6699.04	6686.30	6351.98	334.31	12.74
CH_3OH	14.29	1231.94	15.04	14.29	0.75	1216.89
H_2O	3.13	1220.77	3.29	3.13	0.16	1217.48

Analysis: The molar flow rate of H_2O and CH_3OH in stream 5 is very low, since it mostly contains vapour only. Whereas the molar flow rate of CO_2 and H_2 is vey low in stream 6 which shows this stream mostly contains liquid phase.

The following snapshot is of the command window,

```
Command Window
  Molar flow rates of stream 3 : CO2=4058.8261 H2=10351.9883 CH3OH=14.2958 H2O=3.1317
  Molar flow rates of stream 4 : CO2=2841.1783 H2=6699.0448 CH3OH=1231.9436 H2O=1220.7795
  Molar flow rates of stream 5 : CO2=2167.1854 H2=6686.3035 CH3OH=15.0482 H2O=3.2965
  Molar flow rates of stream 6 : CO2=673.9929 H2=12.7413 CH3OH=1216.8954 H2O=1217.483
  Molar flow rates of recycle stream 5R : CO2=2058.8261 H2=6351.9883 CH3OH=14.2958 H2O=3.1317
  Molar flow rates of stream 5P : CO2=108.3593 H2=334.3152 CH3OH=0.75241 H2O=0.16482
fx >>
```

CONCLUSION

Iteration is a convenient way of finding the molar flow rates of each component in every stream. Such a method can give answer very close to actual value. Also recycle stream helps in saving additional cost by recovering 95% of the vapour phase stream.

APPENDIX

The MATLAB code to solve the problem is as follows:

```
P=7800000;
T=273+40;

K_co2=exp(22.36-(1992.9/T))/P;
K_h2=1.44e9/P;
K_ch3oh=exp(24.8785-(4521.7104/T))/P;
K_h2o=exp(24.70-(4941.25/T))/P;
K = [K_co2 K_h2 K_ch3oh K_h2o];

tol=1e-6;
r=[1000 1000 1000 1000];
diff = 1000000;
```

```matlab
while diff>tol
a = [r(1)+2000 r(2)+4000 r(3) r(4)];  % a1, a2, a3, a4 is for CO2, H2, CH3OH and H2O respectively
b = [0.7*a(1) a(2)-0.9*a(1) 0.3*a(1)+a(3) 0.3*a(1)+a(4)];
F = b(1)+b(2)+b(3)+b(4);
z = b./F;
shi_func = @(s) (sum(z.*(1-K)./(1+s.*(K-1))));
shi = fsolve(shi_func,1);
V = shi*F;
L = F-V;
x = z./(1+shi.*(K-1));
y = x.*K;
d = x.*L;
c = y.*V;
rec= 0.95.*c;
diff = norm(rec-r);
r = rec;
end

disp(['Molar flow rates of stream 3 : CO2=',num2str(a(1)), ' H2=',num2str(a(2)), ' CH3OH=',
num2str(a(3)), ' H2O=', num2str(a(4))])
disp(['Molar flow rates of stream 4 : CO2=',num2str(b(1)), ' H2=',num2str(b(2)), ' CH3OH=',
num2str(b(3)), ' H2O=', num2str(b(4))])
disp(['Molar flow rates of stream 5 : CO2=',num2str(c(1)), ' H2=',num2str(c(2)), ' CH3OH=',
num2str(c(3)), ' H2O=', num2str(c(4))])
disp(['Molar flow rates of stream 6 : CO2=',num2str(d(1)), ' H2=',num2str(d(2)), ' CH3OH=',
num2str(d(3)), ' H2O=', num2str(d(4))])
disp(['Molar flow rates of recycle stream 5R : CO2=',num2str(r(1)), ' H2=',num2str(r(2)), '
CH3OH=', num2str(r(3)), ' H2O=', num2str(r(4))])
disp(['Molar flow rates of stream 5P : CO2=',num2str(c(1)-r(1)), ' H2=',num2str(c(2)-r(2)), '
CH3OH=', num2str(c(3)-r(3)), ' H2O=', num2str(c(4)-r(4))])
```