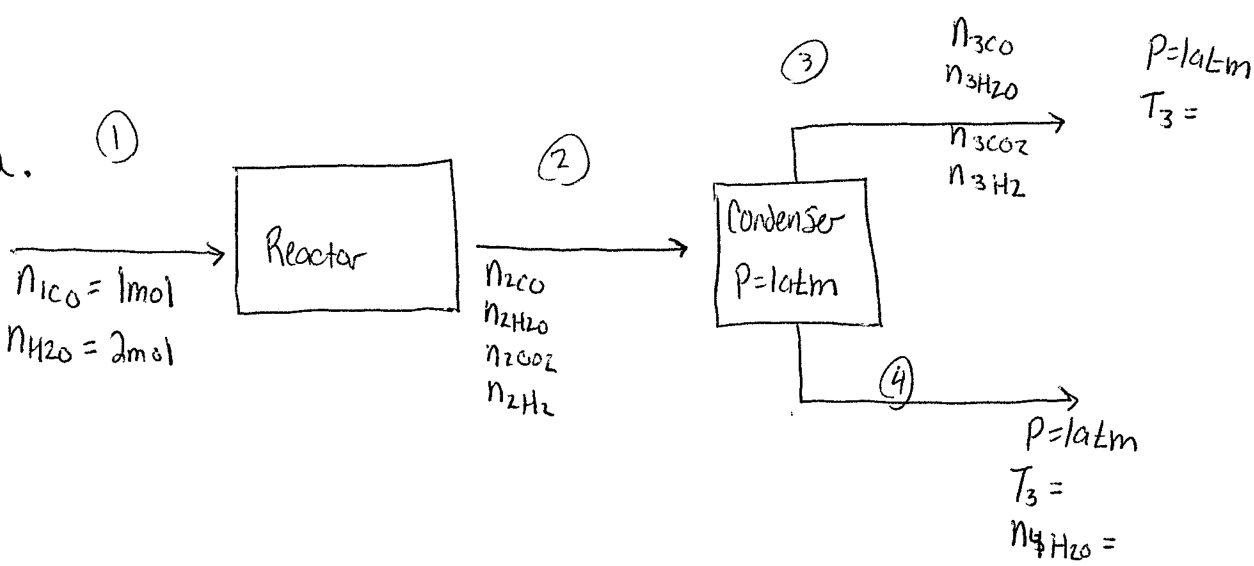
Started in class on
10|17|2018

Practice Problem Solution

$$CO + H_2O \rightleftharpoons CO_2 + H_2$$

a.



b. Composition leaving the reactor: n_{2CO} n_{2H_2O} n_{2CO_2} n_{2H_2}
Temp. of Condenser T_3
Flowrate leaving condenser n_{4H_2O}

c. $$K = 1 = \frac{n_{2CO_2}\, n_{2H_2}}{n_{2CO}\, n_{2H_2O}}$$

$$y_{3H_2O} = 0.20 = \frac{n_{3H_2O}}{n_{3CO} + n_{3H_2O} + n_{3CO_2} + n_{3H_2}}$$

d. DOF on Reactor

4 unknowns (n_{2CO} n_{2H_2O} n_{2CO_2} n_{2H_2O})
+1 reaction
-4 independent material balances
-1 additional equation $\left(K = 1 = \frac{n_{3H_2O}}{n_{3CO} + n_{3H_2O} + n_{3CO_2} + n_{3H_2}} \right)$

0 DOF

DOF Overall

5 unknowns (n_{3CO} n_{3H_2O} n_{3CO_2} n_{3H_2} n_{4H_2O})
+1 reaction
-4 independent material balances
0 additional equations

2 DOF

DOF Condenser

10 unknowns (n_{2CO} n_{2H_2O} n_{2CO_2} n_{2H_2} n_{3CO} n_{3H_2O} n_{3CO_2} n_{3H_2} n_{4H_2O}) T_3
+ 0 reactions
- 4 independent material balances
- 2 additional equations $\left[y_{H_2O} P = P_{H_2O}^{sat} = \log_{10} \left(A - \frac{B}{T+C} \right) \right]$

4 DOF

can be written in terms of n's and $y_{H_2O} = 0.20$

The second quation is the Equilibrium Constant, K

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e. POA: Reactor $\rightarrow$ Condenser

$\boxed{\text{Solve the material balance around the reactor using the following equations!}}$

CO_2: $n_{2CO_2} = 0 + \xi$

H_2: $n_{2H_2} = 0 + \xi$

CO: $n_{2CO} = n_{1CO} - \xi$

H_2O: $n_{2H_2O} = n_{1H_2O} - \xi$

and $K = \dfrac{n_{2CO_2} n_{2H_2}}{n_{2CO} n_{2H_2O}} = 1 = \dfrac{\xi^2}{(\underset{\text{Known}}{n_{1CO}} - \xi)(\underset{\text{Known}}{n_{1H_2O}} - \xi)}$

I would solve K expression for ξ then calculate n_{1CO} and n_{1H_2O} and all n_2's - this tells us the composition of the reactor effluent!

$\boxed{\text{Solve the material balance around the condenser because now we know } (n_{2CO}\ n_{2H_2O}\ n_{2CO_2}\ n_{2CO}) \text{ so DOF} = 0}$

Raoult's Law with the Antoine Equation:

$$\underset{\text{Known}}{y_{3H_2O}} \underset{\text{Known, P=1atm}}{P} = P_{H_2O}^{sat} = \log_{10}\left(A - \frac{B}{T+C}\right)$$

We can solve Raoult's Law directly for T_2!

CO_2: $n_{3CO_2} = n_{2CO_2}$ ✓

H_2: $n_{3H_2} = n_{2H_2}$ ✓

CO: $n_{3CO} = n_{2CO}$ ✓

H_2O: $n_{3H_2O} + n_{4H_2O} = n_2 H_2O$ ✓

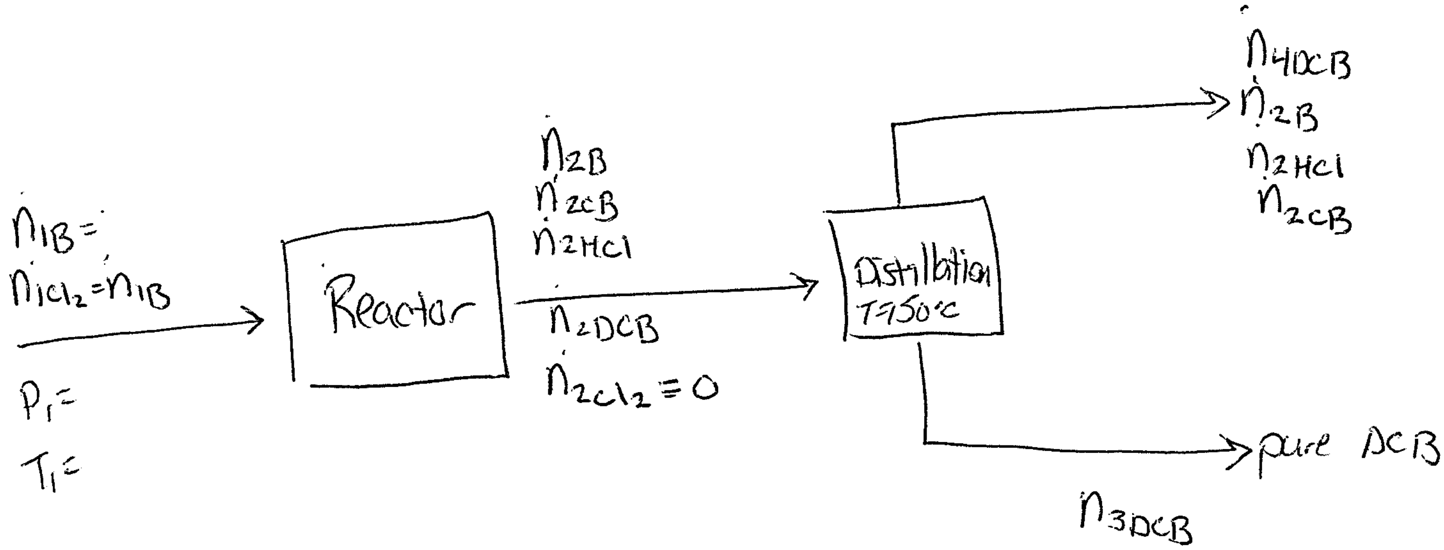
We can use the $y_{3H_2O} = \dfrac{n_{3H_2O}}{\Sigma n_{3i}} = 0.2$

- Solve for n_{3CO_2}, n_{3H_2}, n_{3CO} from the species balances
- Then use vapor phase mol fraction $y_{3H_2O} = 0.2$ equation to solve for n_{3H_2O}
- Then, water balance to calculate $\boxed{n_{4H_2O}}$

Practice Problem 2

$B + Cl_2 \rightarrow CB + HCl$

$B + 2Cl_2 \rightarrow DCB + 2HCl$



$\alpha_{CB/DCB} = 10 = \frac{n_{2CB}}{n_{2DCB}}$

assume a basis, ~~[illegible]~~

$\dot{n}_{2CB} = 100 \frac{mol}{min}$

$y_{DCB} = \frac{n_{DCB}}{\sum n_{4i}}$

$\boxed{\text{Want to know } \dot{V}_{Cl_2} \ \dot{V}_3 \ P_{column}}$

DOF Reactor

4 unknowns ($\dot{n}_{2B}$ $\dot{n}_{2CB}$ $\dot{n}_{2HCl}$ $\dot{n}_{2DCB}$)

+2 reactions

− 5 ind. mat balances (B CB HCl DCB Cl_2)

−1 add. equation ($\alpha_{CB/DCB}$)

0 DOF

Material Balances on the Reactor

B: $\dot{n}_{2B} = \dot{n}_{1B} - \xi_1 - \xi_2$

Cl_2: $0 = \dot{n}_{1Cl_2} - \xi_1 - 2\xi_2$

~~$\dot{n}_{2CB}$~~ CB: $\dot{n}_{2CB} = \xi_1$

HCl: $\dot{n}_{2HCl} = \xi_1 + 2\xi_2$

DCB: $\dot{n}_{2DCB} = \xi_2$

We know:

$$10 = \frac{\dot{n}_{2CB}}{\dot{n}_{2DCB}}$$

$$\dot{n}_{Cl_2} = \dot{n}_{1B}$$

basis $\rightarrow$ $\dot{n}_{2CB} = 100$ mol

1. Calculate ξ_1 from $\underline{\dot{n}_{2CB}}$ eq.
2. Calculate $\dot{n}_{2DCB}$ from α equation
3. Calculate ~~m~~ ξ_2 using DCB balance
4. Calculate $\dot{n}_{1Cl_2}$ using Cl_2 balance
5. Calculate $\underline{\dot{n}_{1B}}$ from feed ratio.
6. Use $\dot{n}_{1B}$ in B balance to calculate $\dot{n}_{2B}$

~~$\dot{n}_{1B}$ can be used to calculate~~

Now we know all $\dot{n}_{2i}$ .... so we can use these in the distillation calculations to get $\dot{n}_{3DCB}$ (and eventually

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Material Balances on distillation column

in=out b/c non-reactive subsystem

DCB: $n_{2DCB} = n_{4DCB} + n_{3DCB}$ and $y_{DCB} = 0.8 = \frac{n_{4DCB}}{n_{2DCB} + n_{2CB} + n_{2B} + n_{4DCB}}$

1. We know ~~[illegible]~~ n_{2CB} n_{2HCl} n_{2B} from reacter calcs, so we can use $y_{DCB} = 0.8$ to calculate n_{4DCB}
2. Use n_{4DCB} in DCB balance to calc. n_{3DCB}.

Calc. $\dot{V}_3$

$$\frac{\dot{n}_{3DCB}\left(\frac{mol}{min}\right) \cdot MW_{DCB}\left(\frac{g}{mol}\right)}{\rho_{DCB}\left(\frac{g}{L}\right)} = \dot{V}_3\left(\frac{L}{min}\right)$$

* look up MW_{DCB}, ρ_{DCB}

Calc. $\dot{V}_{1Cl_2}$

$$P_1 V_1 = n_{1Cl_2} R T_1$$

$$V_{1Cl_2} = \frac{n_{1Cl_2} R T_1}{P_1}$$

and $P_1 = 1\,atm$

$T_1 = 100°C \rightarrow$ convert to K

373 K

$n_{1Cl_2} \rightarrow$ calculated from reacto balances.

~~[illegible]~~

Calc P_{column}

$y_{DCB} P = P_{DCB}^{sat}$

via Antoine $P_{DCB}^{sat} = 10^{\left[A - \frac{B}{T+C}\right]}$

given