Conceptual Questions

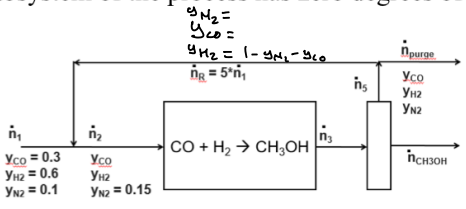
1. (5 points) Consider the reaction 2A + B → 2C in a steady state, continuous flow reactor. The feed contains 100 mol A/s, 200 mol B/s and 50 mol C/s. What is the flowrate of C exiting the reactor if A is consumed at a rate of 5 mol/s?
   a. 5 mol/s
   b. 10 mol/s
   c. 55 mol/s
   d. 60 mol/s
   e. 150 mol/s

$5\ \text{mol A/s} \times \frac{2\ \text{mol C}}{2\ \text{mol A}} = 5\ \text{mol C/s}$

$C_{out} = C_{in} + \text{Generation} - \text{Consumption}$ (C is not being reacted)

$\rightarrow C_{out} = 50\ \text{mol/s} + 5\ \text{mol/s} = 55\ \text{mol/s}$

2. (5 points) Which subsystem of the process has zero degrees of freedom?



   a. Mixing point
   b. Reactor
   c. Condenser
   d. Overall balance
   e. None of the above

Assuming n_1 basis brings min {DoF} to 1 only !!

Mixing Point

7 Unknowns ($2y_{2i}$, $2y_{Ri}$, $\dot{n}_1$, $\dot{n}_2$, $\dot{n}_R$)
3 Indep Mat Blncs (CO, H_2, N_2)
−2 Additional EQs ($\dot{n}_R = 5\dot{n}_1$, $0.85 = y_{CO} + y_{H_2}$)
2 DoF !!

Reactor

7 Unknowns ($2y_{2i}$, $3y_{3i}$, $\dot{n}_2$, $\dot{n}_3$)
−4 Indep Mat Blncs (4 species)
−0 Additional EQs
+1 Indep Chem Rxns ($\dot{\xi}$)
4 DoF !!

Condenser

9 Unknowns ($\dot{n}_{CH_3OH}$, $\dot{n}_3$, $\dot{n}_5$, $3y_{3i}$, $3y_{5i}$)
−4 Indep Mat Blncs (4 species)
−1 Additional EQs ($y_{N_2} = 1 - y_{CO_2} - y_{H_2}$)
4 DoF !!

Overall

6 Unknowns ($\dot{n}_1$, $\dot{n}_{CH_3OH}$, $\dot{n}_{purge}$, $3y_{3i}$)
4 Indep Mat Blncs (4 species)
−1 Additional EQs ($y_{N_2} = 1 - y_{CO_2} - y_{H_2}$)
+1 Indep Chem Rxns ($\dot{\xi}_{overall}$)
2 DoF !!

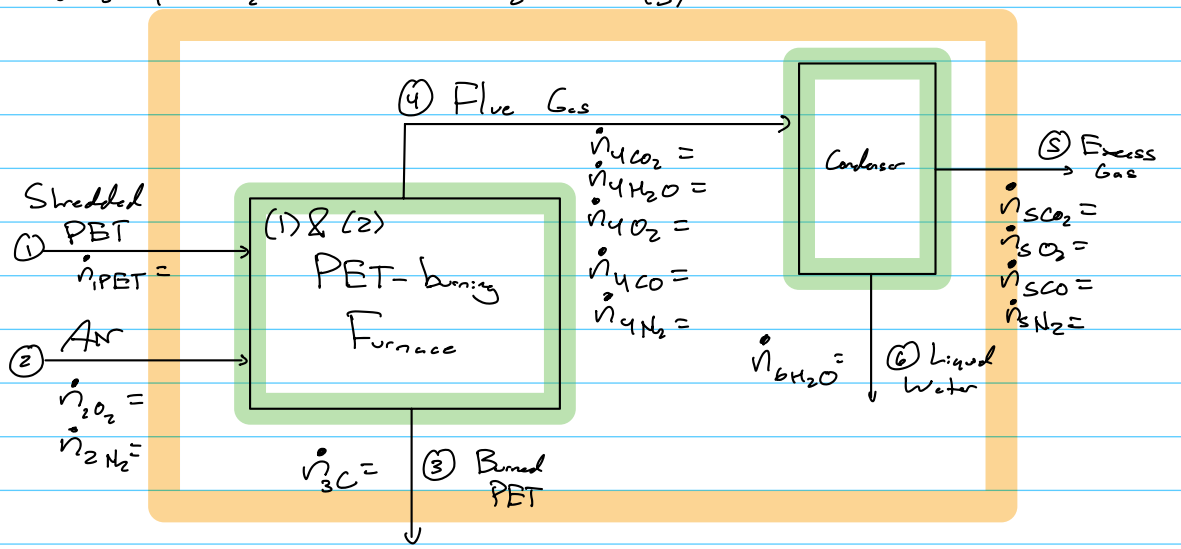
3) Waste Management Carbon Emission Analysis

(1) $C_{10}H_8O_4 + 9O_2 \rightarrow 9CO_2 + 4H_2O + C(s)$

(2) $C_{10}H_8O_4 + 4O_2 \rightarrow 8CO + 4H_2O + 2C(s)$

Note: $C_{10}H_8O_4$ is labeled below as PET

A)



Additional Info

$f_{PET} = 1 = \frac{\dot{n}_{3C}}{\dot{n}_{1PET}}$

$a_{\frac{CO}{CO_2}} = 4 = \frac{\dot{n}_{4CO}}{\dot{n}_{4CO_2}}$

Additional EQs

① $\frac{\dot{n}_{2O_2}}{\dot{n}_{1PET}} = \frac{3}{1}$, ② $\frac{\dot{n}_{2O_2}}{\dot{n}_{2O_2} + \dot{n}_{2N_2}} = 0.21$

③ $4\dot{n}_{4CO_2} = \dot{n}_{4CO}$

Want to Know: $f_{O_2,single} = \frac{\dot{n}_{2O_2} - \dot{n}_{4O_2}}{\dot{n}_{2O_2}}$ Need: $\dot{n}_{2O_2}, \dot{n}_{4O_2}$

DoF Analysis

Furnace

9 Unknowns ($\dot{n}_{1PET}, \dot{n}_{2O_2}, \dot{n}_{2N_2}, \dot{n}_{3C}, S\dot{n}_{4i}$)
- 7 Indep Mat Balances (CO_2, H_2O, O_2, CO, N_2, C, PET)
- 3 Additional EQs (①, ②, ③)
+ 2 Indep Chemical Equations ($\dot{\xi}_1, \dot{\xi}_2$)
1 DoF

Condenser

10 Unknowns ($\dot{n}_{6H_2O}, S\dot{n}_{4i}, 4\dot{n}_{5i}$)
- 5 Indep Mat Balances (CO_2, CO, N_2, O_2, H_2O)
- 1 Additional EQ (③)
+ 0 Chemical Rxns
4 DoF !!

Overall

9 Unknowns ($\dot{n}_{1PET}, \dot{n}_{2O_2}, \dot{n}_{2N_2}, \dot{n}_{3C}, \dot{n}_{6H_2O}, 4\dot{n}_{5i}$)
- 7 Indep Mat Balances (PET, O_2, N_2, C, CO_2, CO, H_2O)
- 2 Additional EQs (①, ②)
+ 2 Indep Chemical Reactions ($\dot{\xi}_1, \dot{\xi}_2$)
2 DoF

Assume a basis of $\dot{n}_{1PET} = 100$ mol/hr so Furnace gas to 0 DoF. Solvable!

Waste Management Carbon Emission Analysis (Continued)

Material Balances

0 accumulation, cts. & steady-state

Furnace

out = in + gen/cons

CO_2: $\dot{n}_{4CO_2} = 0 + 9\dot{\xi}_1$

H_2O: $\dot{n}_{4H_2O} = 0 + 4\dot{\xi}_1 + 4\dot{\xi}_2$

O_2: $\dot{n}_{4O_2} = \dot{n}_{2O_2} - 9\dot{\xi}_1 - 4\dot{\xi}_2$

N_2: $\dot{n}_{4N_2} = \dot{n}_{2N_2} \pm 0$ nonreactive

CO: $\dot{n}_{4CO} = 0 + 8\dot{\xi}_2$

C: $\dot{n}_{3C} = 0 + \dot{\xi}_1 + 2\dot{\xi}_2$

PET: $0 = n_{1PET} - \dot{\xi}_1 - \dot{\xi}_2$

Condenser

in = out

no accumulation & no reaction here

CO_2: $\dot{n}_{4CO} = \dot{n}_{5CO}$

H_2O: $\dot{n}_{4H_2O} = \dot{n}_{6H_2O}$

O_2: $\dot{n}_{4O_2} = \dot{n}_{5O_2}$

N_2: $\dot{n}_{4N_2} = \dot{n}_{5N_2}$

CO: $\dot{n}_{4CO} = \dot{n}_{5CO}$

Total: $\sum \dot{n}_{4i} = \dot{n}_{6H_2O} + \sum \dot{n}_{5i}$ ← Not useful but written for brevity

0 accumulation, cts. & steady-state

Overall

out = in + gen/cons

CO_2: $\dot{n}_{5CO_2} = 0 + 9\dot{\xi}_1$

H_2O: $\dot{n}_{6H_2O} = 0 + 4\dot{\xi}_1 + 4\dot{\xi}_2$

O_2: $\dot{n}_{5O_2} = \dot{n}_{2O_2} - 9\dot{\xi}_1 - 4\dot{\xi}_2$

N_2: $\dot{n}_{5N_2} = \dot{n}_{2N_2}$

CO: $\dot{n}_{5CO} = 0 + 8\dot{\xi}_2$

C: $\dot{n}_{3C} = 0 + \dot{\xi}_1 + 2\dot{\xi}_2$

PET: $0 = \dot{n}_{1PET} - \dot{\xi}_1 - \dot{\xi}_2$

B) Want to know: $f_{O_2,\text{stoic}} = \frac{\dot{n}_{2O_2} - \dot{n}_{4O_2}}{\dot{n}_{2O_2}}$

(need $\dot{n}_{2O_2}, \dot{n}_{4O_2}$)

How to solve: Solve Furnace "

(i) Solve ① for $\dot{n}_{2O_2}$

(ii) Use ② to substitute $4\dot{n}_{4CO_2} = \dot{n}_{4CO}$ into CO balance and recurse to $\dot{n}_{4CO_2} = 2\dot{\xi}_2$ (*)

(iii) Substitute (*) into CO_2 balance to get a ratio of $\dot{\xi}_i$ as

$2\dot{\xi}_2 = 9\dot{\xi}_1 \rightarrow \frac{2}{9} = \frac{\dot{\xi}_1}{\dot{\xi}_2}$ (**)

(iv) Solve (**) for $\dot{\xi}_1$ in terms of $\dot{\xi}_2$ and plug in to PET balance to solve for $\dot{\xi}_2$

(v) Solve PET balance for $\dot{\xi}_1$ ← Can now solve for both intermediates

(vi) Solve O_2 balance for $\dot{n}_{4O_2}$

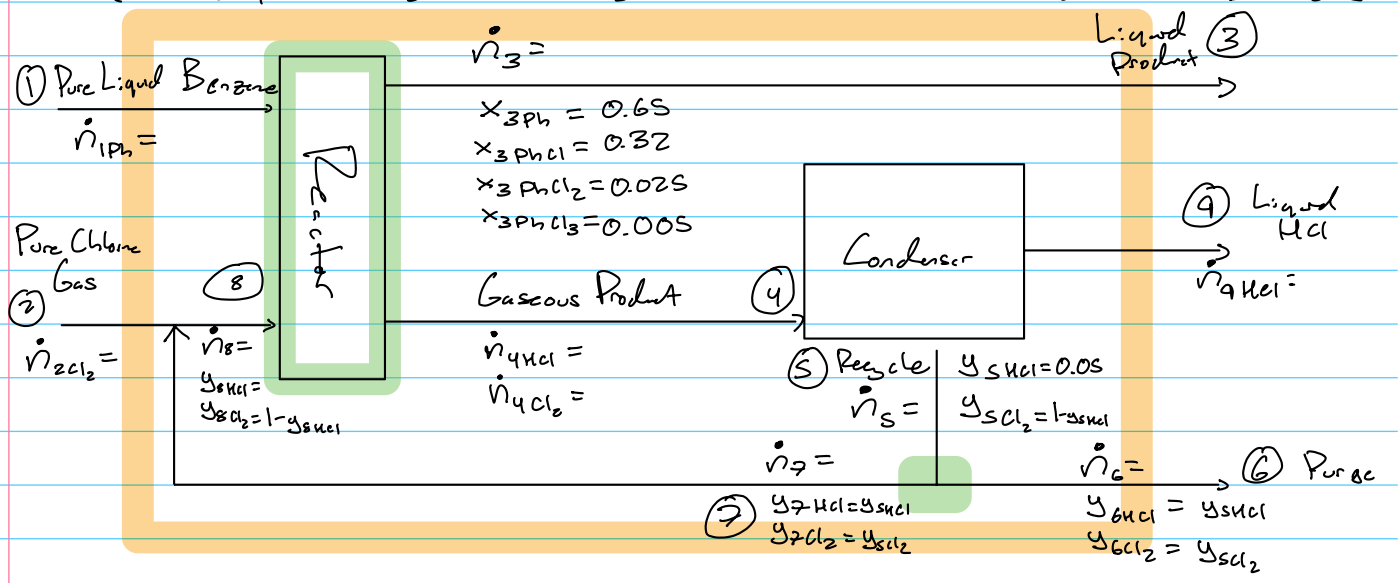
Now we have $\dot{n}_{2O_2}$ & $\dot{n}_{4O_2}$ to find $f_{O_2,\text{stoic}} = \frac{\dot{n}_{2O_2} - \dot{n}_{4O_2}}{\dot{n}_{2O_2}}$ as required.

4) Chlorobenzene Production

A) (1) $C_6H_6 + Cl_2 \xrightarrow{Catalyst} C_6H_5Cl + HCl$ Assume: Catalyst is 'not present'

(2) $C_6H_5Cl + Cl_2 \xrightarrow{Catalyst} C_6H_4Cl_2 + HCl$ Left: Ph: C_6H_6 $PhCl_2$: $C_6H_4Cl_2$

(3) $C_6H_4Cl + Cl_2 \xrightarrow{Catalyst} C_6H_3Cl_3 + HCl$ PhCl: C_6H_5Cl $PhCl_3$: $C_6H_3Cl_3$



Want to Know: $f_{Ph,single} = \frac{\dot{n}_{1Ph} - \dot{n}_3 x_{3Ph}}{\dot{n}_{1Ph}} = f_{Ph,overall}$, $\alpha_{\frac{PhCl}{PhCl_2}} = \frac{\dot{n}_3 x_{3PhCl}}{\dot{n}_3 x_{3PhCl_2}}$ Need: $\dot{n}_{1Ph}, \dot{n}_3$

B) DoF Analysis (just for purge & reactor)

Purge

3 Unknowns ($\dot{n}_5, \dot{n}_6, \dot{n}_7$)
2 Indep Mat Balances (Cl_2, HCl)
− 0 Additional EQs
+ 0 Chemical Rxns
1 DoF

Reactor

6 Unknowns ($\dot{n}_{1Ph}, \dot{n}_8, y_{8HCl}, \dot{n}_3, \dot{n}_{4HCl}, \dot{n}_{4Cl_2}$)
6 Indep Mat Balances (Ph, PhCl, $PhCl_2$, $PhCl_3$, HCl, Cl_2)
− 0 Additional EQs
+ 3 Chemical Rxns ($\dot{\xi}_1, \dot{\xi}_2, \dot{\xi}_3$)
3 DoF

C) Material Balances (just for Cl_2 in reactor & overall)

Out = in + gen/cons No accumulation, Reactor Process

$\rightarrow \dot{\xi}_j \neq \dot{\xi}_{j,overall}$ as there is a recycle stream!

Reactor

Cl_2: $\dot{n}_{4Cl_2} = \dot{n}_8 y_{8Cl_2} - \dot{\xi}_1 - \dot{\xi}_2 - \dot{\xi}_3$

Overall

Cl_2: $\dot{n}_{2Cl_2} = \dot{n}_6 y_{6Cl_2} - \dot{\xi}_{1,overall} - \dot{\xi}_{2,overall} - \dot{\xi}_{3,overall}$

Reflection Question

4. We have now finished unit 3 on material balances for system with chemical reactions.
    a. How did you study for Quiz 1?
    b. What concepts (if any) are unclear or do you struggle with?

(A) For quiz 1, I studied by reviewing all of the in class examples and homework assignments. To do this, I copied the problem statements to a different file and solved each of them 'cold-turkey' as suggested. I would then go through and check my work and correct anything that I had gotten wrong. Importantly, I also went through all of the 'Test-Yourself' sections in the textbook. This was because the examples in class were not conceptual based, and I wanted to get practice with multiple-choice style answers as well. The other thing I did to study was reviewing the homework feedback I got, and redoing the Hemodialysis problem from HW2B. I chose to redo this problem specifically because it gave me a lot of trouble when I solved it the first time. In summary, I studied by reviewing all of the accessible materials given to me, which allowed me to feel confident going into the quiz.

(B) Currently, I'm struggling with differentiating between single and overall fractional conversions. While this isn't giving me too much trouble, it is something that I need to work on and get used to more as the semester goes on. Other than that, the only other thing that confuses me sometimes is the problem statements, as the wording sometimes trips me up and I overthink what information is given. This is more of something I just have to get used to as I familiarize myself with the ever increasing amount of jargon in this class. I'm feeling a lot more comfortable drawing PFDs and properly labeling them when compared to how I felt after HW2A.