Unit 1

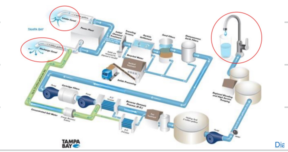
Unit 1: Units and Process Variables

Process Variables

Def: A value or parameter which can be monitored or measured or controlled in a given system

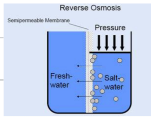
① Salt Water Desalination

Tampa Bay Distillation



Large Scale thermal distillation way too energy and cost intensive

SW Reverse Osmosis: Membrane separation process through semi-permeable, selective membrane. Large pressure applied opposite to natural osmosis



We simplify to a process flow diagram to allow us to ignore actual machine.

Process Flow Diagram for desalination

Feed → Desalination Process (Separator) → Product

x_{NaCl} (g NaCl / g Seawater)

↓ Reject (brine)

Relevant Process Variables ← For systems to the right

- Composition
  - mass fraction: $\frac{\text{mass of } i}{\text{mass of mixture}} = x_i$ (for liquids) or y_i (for gases/vapor)
  - mol fraction: $\frac{\text{mol of } i}{\text{moles of mixture}} = x_i$ or y_i
- Pressure, P
- Flow Rates
  - Mass Flowrate, $\dot{m}$ $\left(\frac{\text{mass}}{\text{time}}\right)$
  - Volumetric Flowrate, $\dot{V}$ $\left(\frac{\text{volume}}{\text{time}}\right)$
  - Molar Flowrate, $\dot{n}$ $\left(\frac{\text{mols}}{\text{time}}\right)$
  - Energy Flowrate, $\dot{H}$ $\left(\frac{\text{energy}}{\text{time}}\right)$
- Temperature, T

→ Flowrate Calculations

The desalination plant produces 25 million gallon per day of drinking water.

$\dot{V} = 25{,}000{,}000$ ← 2 sig figs

What is the mass flowrate of drinking water? $\dot{m}$ in $\frac{\text{lbs}}{\text{day}}$

america density of water: 8.33 lbs/gal

$$\frac{25{,}000{,}000 \text{ gal}}{1 \text{ day}} \times \frac{8.33 \text{ lbs}}{1 \text{ gal}} = \boxed{210{,}000{,}000 \ \frac{\text{lbs}}{\text{day}} = \dot{m}}$$

2 sig figs

If calculating and looking up online, truncate as needed but use as many digits as possible. Also, round sig-figs on final answer ☺

What is the molar flowrate of drinking water? $\dot{n}$ in $\frac{\text{mols}}{\text{day}}$

$$\frac{25{,}000{,}000 \text{ gal}}{1 \text{ day}} \times \frac{8.33 \text{ lbs}}{1 \text{ gal}} \times \frac{1 \text{ Kg}}{2.2046 \text{ lbs}} \times \frac{1000 \text{ g}}{1 \text{ Kg}} \times \frac{1 \text{ mol}}{18.02 \text{ g}} = \boxed{5.3 \times 10^{9} \ \frac{\text{mol}}{\text{day}} = \dot{n}}$$

Salinity of seawater by mass is 3.5%. What is the mol fraction of salt (NaCl)?

Suppose 100 g seawater are present

Assume Basis

$$3.5 \text{ g NaCl} \times \frac{1 \text{ mol NaCl}}{58.04 \text{ g}} = \text{mol NaCl}$$

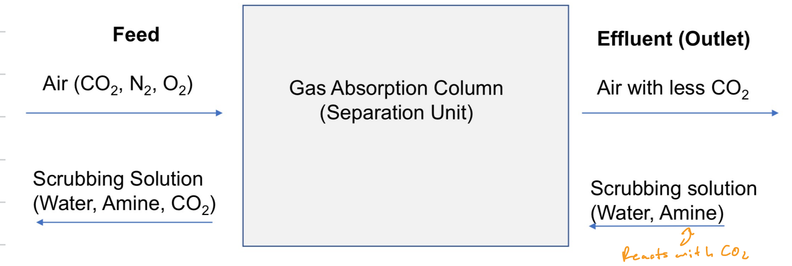
$$96.5 \text{ g } H_2O \times \frac{1 \text{ mol } H_2O}{18.02 \text{ g}} = \text{mol } H_2O$$

$$x_{NaCl}\left(\frac{\text{mol NaCl}}{\text{mol Seawater}}\right) = \frac{n_{NaCl}}{n_{NaCl} + n_{H_2O}}$$

(2) CO_2 Capture

Chemical Engineers can design pollution control Systems (absorbers/membranes) to remove CO_2 from industrial waste

Gas absorption columns: Use reactions to capture CO_2 for use in chemical synthesis



Relevant Process Variables

Individual Discussion
- Air Pressure
- Amine : CO_2 Ratios
  - ↳ Solution Concentration
- Fraction CO_2 Removed

Group Discussion
- Flowrate ($\dot{m}_i$, $\dot{n}_i$, $\dot{V}_i$) i = species
  - ↳ Total Flowrate ($\dot{m}$, $\dot{n}$, $\dot{V}$)
- Composition of each stream (x_i vs. y_i) gases
- Energy Flowrates ($\dot{H}$)
- Temperature and Pressure

Assume air behaves ideally and enters the absorber with $\dot{n}_1 = 1$ mol/min.

Write an equation for $\dot{V}_1$

$P_1 V_1 = n_1 R T_1$ and $P\dot{V} = \dot{n} R T$ is also valid

Be specific about stream which is ideal

$$\boxed{\rightarrow \dot{V}_1 = \frac{\dot{n}_1 R T_1}{P_1}}$$

Consider air is a mixture of CO2, N2, O2. By mass: 76.95% N2, 0.05% CO2, and 23% O.

Weighted Average Property of a mixture: $MW_{air}\ (g/mol) = \sum y_i MW_i$ ← molar masses of all species i

↑ mol fractions of all species i

$\therefore MW_{air}\ (g/mol) = y_{N_2} MW_{N_2} + y_{CO_2} MW_{CO_2} + y_{O_2} MW_{O_2}$

Process for Solving

(i) Look up all MW

(ii) Convert mass fraction to mol fraction for all species

Assume a basis for your calculations: 100 g air

Unit 2

Unit 2: Fundamentals of Material Balances on Non-Reactive Processes

Types of Reactors

Batch: Reactants fed to reactor at beginning and removed later. No mass crosses system boundary

Allows for 'bad batches'

Examples: Beverage fermentation, Pharmaceuticals, and Food Production

Continuous: Reactants and Products continuously flow in and out of the reactor

Examples: Large-scale food production (Blending processes, polymer extruders)
Commodity chemical Production

Faster and 24/7 processes, worker safety due to sealed facilities

Semi-batch: Partly batch and partly continuous

Examples: Polymerization reactions, Exothermic reactions (Diluting Reactions)

Steady-State vs. Transient Processes

we do this type in this class

(1) Steady-State: Process variables ~~do~~ not change with time with cts. processes

(2) Transient: Process variable change with cts. process

↳ require differential equations

Material Balance: in − out + accumulation − consumption = 0

General problem solving procedure: Material balances on non-reactive systems

→ □ →

watch for these mostly

1. Draw and label a process flow diagram (PFD)
   - Label All streams with <u>Known</u> process variables (T, P, x_i/y_i, $\dot{m}$, ...)
   - Label All streams with <u>Unknown</u> process variables
   - Identify quantities for which you will solve

2. Perform a degree of freedom analysis on each subsystem

     # unknown process variables
   − # independent material balances   *max will be # of species in your subsystem
   − # additional mathematical relationships

   DOF

   If DOF ≤ 0, then... solve!

   If DOF > 0, then... Cannot solve... ← This is a reasonable answer

3. Convert all quantities to the same basis

4. Determine the “plan of attack” (POA): the order that you will solve the subsystems

5. Write all material balances for all necessary subsystems

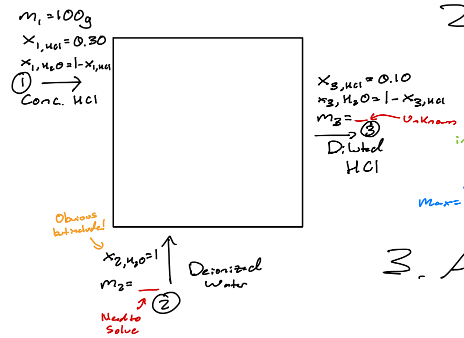
6. Identify the equations you will use to solve for the desired quantities and the order in which you will solve them.

7. SOLVE! Now, you can plug in numbers to calculate quantitative answers

SINGLE UNITS

<u>Example 1: Diluting HCl</u>. In a batch mixing process at a chemical plant, 100g of 30wt% HCl is diluted with deionized water. The final product is 10wt% HCl. How much water is needed for this process?

1.



Want to Know: m_2

2. Degree of Freedom (DoF) Analysis

→ unknowns (m_2, m_3) Include even if not solution

Derived from law of cons. of mass: → Independent Material balances: 2

Can write 2 many as there are 2 species (HCl + H_2O)

→ 0 additional equations

in − out + gen − cons. = accumulation

Max = # species!

$2 - 2 - 0 = 0$ DOF (Y)

unknowns mat. bal. additional eqs.

3. All Process variables on same basis?

↳ Are we dimensionally consistent? ✓

4. Material Balances

(gen) (cons.)

in − out + ~~generation~~ − ~~consumption~~ = ~~accumulation~~ 0 0 0

No chemical Reaction

Everything exits we have a batch process!

→ in − out = 0 ∴ in = out

5. These are the only indep. ones

HCl: $\underbrace{m_1 x_{1,HCl}}_{g\,HCl} = m_3 x_{3,HCl}$

H_2O: $m_1 x_{1,H_2O} + m_2 x_{2,H_2O} = m_3 x_{3,H_2O}$

Add up indep and cancel out with mass fractions → Total Mass: $m_1 + m_2 = m_3$

$m_1 x_{1HCl} + m_1 x_{1H_2O} + m_2 x_{2H_2O} =$

$m_3 x_{3HCl} + m_3 x_{3H_2O}$

$\to m_1 (\cancel{x_{1HCl} + x_{1H_2O}})^{1} + m_2 \cancel{x_{2H_2O}}^{1} =$

$m_3 (\cancel{x_{3HCl} + x_{3H_2O}})^{1}$

$\to m_1 + m_2 = m_3$

6. Plan of Attack (PoA)

(i) Solve HCl for m_3

(ii) Solve H_2O for m_2 using (i) result

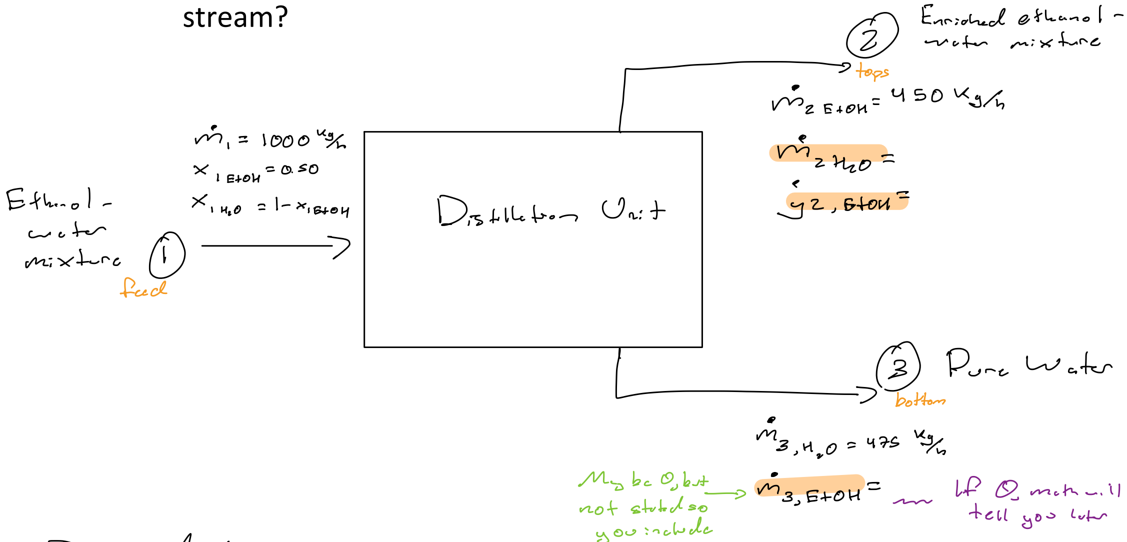
↳ For ease, solve m_2 from mass balance

7. $m_3 = \dfrac{m_1 x_{1HCl}}{x_{1HCl}}$ ↖ Usually stop here on exams

$m_1 + m_2 = \dfrac{m_1 x_{1HCl}}{x_{1HCl}}$

$$\boxed{\to m_2 = \frac{m_1 x_{1HCl}}{x_{1HCl}} - m_1}$$

Example 2: Continuous Distillation. In a continuous, steady state process, 1000 kg/h of 50wt% ethanol/water mixture is separated by distillation. Due to the vapor-liquid equilibrium achieved by ethanol and water, the top stream is enriched in ethanol but still contains some water. The mass flowrate of ethanol in the tops stream is 450 kg ethanol/hour. The mass flowrate of water in the bottom stream is 475 kg water/hour. What is the composition (by mass) of the top stream?



Want to know

Binary Mixture

(★) $y_{2\,EtOH} = \dfrac{\dot{m}_{2\,EtOH}}{\dot{m}_{2\,EtOH} + \dot{m}_{2H_2O}}$

$y_{2H_2O} = 1 - y_{2\,EtOH}$

$\dot{m}_{2H_2O}$ is all we really need

DoF Analysis

Could include or exclude certain ones and still end up being correct

2 Unknowns ($\dot{m}_{2,H_2O}$, $\dot{m}_{3,EtOH}$)

− 2 independent material balances

− 0 additional EQs

0 DoF Yay! Its Solvable!

Potential Unknowns for DoF

3 ($y_{2,EtOH}$, $\dot{m}_{3,EtOH}$, $\dot{m}_{2H_2O}$)

−2 ind mat. balances

−1 EQ ($y_{2,EtOH}$ ★ eq)

All quantities are on a mass basis

Material Balances

Law of conservation of mass

in − out + generation − consumption = accumulation (generation → 0, consumption → 0, accumulation → 0)

No! Physical Separation / no chem rxns

Its Steady-State! So there is 0 accumulation

→ in = out

EtOH: $\underset{\text{kg EtOH/h}}{\dot{m}_1 x_{1,EtOH}} = \underset{\text{kg EtOH/h}}{\dot{m}_{2,EtOH}} + \underset{\text{kg EtOH/h}}{\dot{m}_{3,EtOH}}$

H_2O: $\dot{m}_1 x_{1,H_2O} = \dot{m}_{2,H_2O} + \dot{m}_{3,H_2O}$

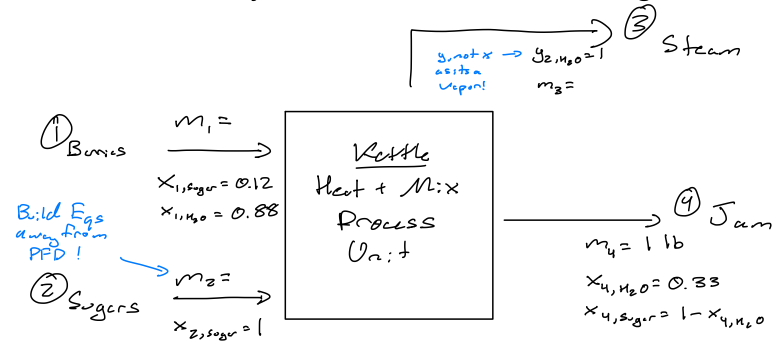
Total: $\dot{m}_1 = \dot{m}_{2,EtOH} + \dot{m}_{2,H_2O} + \dot{m}_{3,EtOH} + \dot{m}_{3,H_2O}$

Plan of Attack

(i) Solve H_2O for $\dot{m}_{2,H_2O}$

(ii) Use $\dot{m}_{2,H_2O}$ in (★) //

Example 3: Strawberry Jam. Strawberries contain 12wt% sugars and 88wt% water. To make jam, crushed strawberries are mixed with additional sugars in a 45:55 mass ratio. Then the mixture is heated until the residue is 1/3 water by mass. How many lbs. of strawberries are needed to make 1 lbs. of jam? How much additional sugar is needed to make 1 lbs. of jam?



Additional EQs

(not derived from law of conservation of mass)

Feed Ratio: $\frac{m_1}{m_2} = \frac{45}{55}$

Want to Know

m_1, m_2

DoF Analysis

3 unknowns (m_1, m_2, m_3)

− 2 independent material balances
(two species, sugar & water)

− 1 additional equation

0 → DoF ≤ 0
Can solve!

Material Balances

Always start with law of conservation of mass!

in − out + ~~gen~~ − ~~consump~~ = ~~accumulation~~
no chemical rxns: gen = 0, consump = 0
Batch process as final quantity is a mass, not flowrate: accumulation = 0

→ in = out

H_2O: $m_1 x_{1,H_2O} = m_3 + m_4 x_{4,H_2O}$

Sugar: $m_1 x_{1,sugar} + m_2 = m_4 x_{4,sugar}$

Total: $m_1 + m_2 = m_3 + m_4$

Independent Balances

Feed Ratio

$\frac{m_1}{m_2} = \frac{45}{55}$

Try Highlighting everything you know

How to Solve

(i) Solve (Feed Ratio) for m_1

(ii) Plug (Feed Ratio) into sugar balance to solve for m_2

(iii) Plug m_2 into (Feed Ratio) to solve m_1

Solve

Not needed on HW unless specified

(i) $m_1 = \frac{45}{55} m_2$

(ii) $\frac{45}{55} m_2 x_{1S} + m_2 = m_4 x_{4S}$

$m_2\left(\frac{45}{55} x_{1S} + 1\right) = m_4 x_{4S}$

$m_2 = \frac{m_4 x_{4S}}{\frac{45}{55} x_{1S} + 1}$

(iii) . . .

Don't need to do the algebra

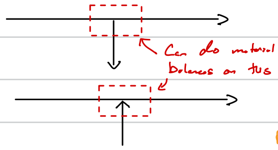
Rm 105

Multi-Unit Processes w/ Recycle and Bypass Streams

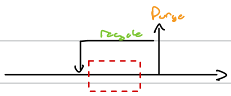
New Terminology

Splitting Point: Where 1 stream becomes 2 streams

Mixing Point: Where 2 or more streams become 1 stream



Purge: When a portion of the recycle stream is split and leaves the system



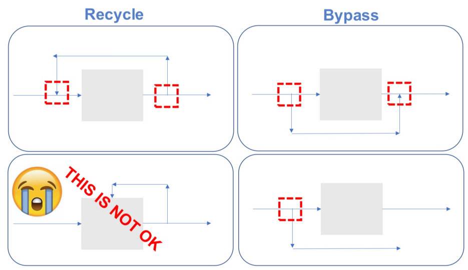
Note

 is a <u>subsystem</u> for all pictures and PFD here

Recycle vs. Bypass

Recycle: Dilute a stream
Circulate a working fluid
Recover a catalyst
Reuse unreacted components

Bypass: circumvent a unit operation
overflow condition for safety

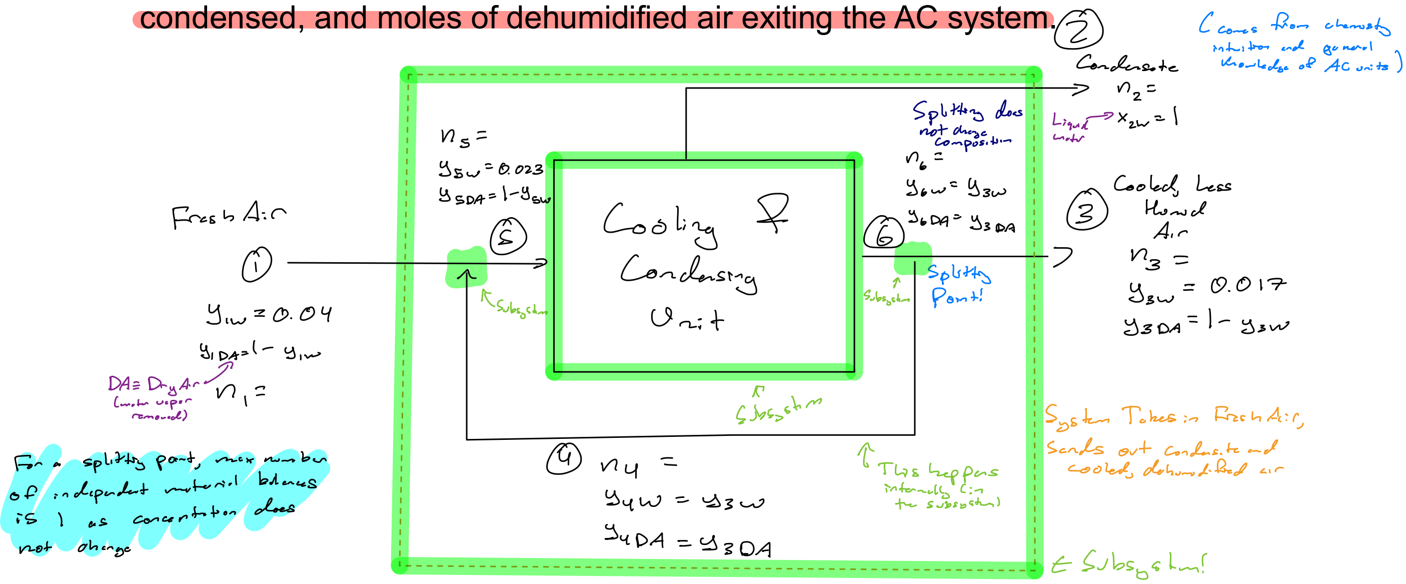


"The stream is recycled into the reactor" means stream recycled into feed going into reactor!

RECYCLE AND BYPASS (SINGLE AND MULTI UNIT)

Example 4: Air conditioning. An air conditioning system takes in fresh air (4mol% water vapor) and outputs cooled air with lower humidity (1.7 mol% water vapor). A stream of fresh air is combined with a recycled stream of cooled/dehumidified air and is passed through the condenser which lowers the humidity and cools the air. The blended air entering the condenser is 2.3mol% water vapor. The air conditioning system operates as a continuous, steady state process. Calculate the moles of fresh feed, moles of water condensed, and moles of dehumidified air exiting the AC system.

Differential Balance



If you are only given compositions, you may assume a basis for your calculation!

Want to Know: n_1, n_2, n_3

units consistent? ✓

DoF Analysis — Can do 1 per subsystem. Can and should do all 4!

Present Subsystems: • Entire (Overall) System, Splitting Point, Mixing Point, cooling/condensing

Overall-DoF: 3 unknowns (n_1, n_2, n_3)
− 2 indep. material balances (W, DA)
− 0 additional EQs ← Cannot be derived from Com on the PFD
1 DoF, cannot solve here!

Given only compositional information, assume a basis after DoF analysis is completed

Mixing-DoF: 3 unknowns (n_1, n_4, n_5)
− 2 indep. material balances (W, DA)
− 0 additional EQs ← Common one here would be like a mixing ratio
1 DoF !!

Given only compositional information, assume a basis after DoF analysis is completed

Splitting-DoF: 3 unknowns (n_3, n_4, n_6)
− 1 indep. material balances ← max 2 as DA & W, but comp is same so we can only write 1 !!
− 0 additional EQs
2 DoF, cannot solve here either!

W: $n_6 y_{6w} = n_4 y_{4w} + n_3 y_{3w}$
DA: $n_6 y_{6DA} = n_4 y_{4DA} + n_3 y_{3DA}$
$\rightarrow n_6 = n_4 + n_3$

Cooling/Condensing-DoF: 3 unknowns (n_2, n_5, n_6)
− 2 indep. material balances (W, DA)
0 additional Equations
1 DoF !!

Only can do it when only compositions are given!

look at subsystems with DoFs 1

Try to avoid assuming a basis for what you're looking to find

Plan
We have to assume a basis,

(i) Go for n_5, as it allows us to solve 2 subsystems
$n_5 = 100$ mol

(ii) Solve cooling/condensing → mixing

(iii) Use splitting to solve for n_3

Material Balances

Highlight as things are known

Cooling / Condensing Mat Balances

W: $n_5 y_{5,w} = n_6 y_{6w} + n_2$

DA: $n_5 y_{5DA} = n_6 y_{6DA}$

Total: $n_5 = n_6 + n_2$

How to Solve:

(i) Solve (DA) for n_6

(ii) Solve (Total) for n_2

Mixing Mat Balances

W: $n_1 y_{1w} + n_4 y_{4w} = n_5 y_{5w}$

DA: $n_1 y_{1DA} + n_4 y_{4DA} = n_5 y_{5DA}$

Total: $n_1 + n_4 = n_5$

How to Solve:

(i) Solve (Total) in terms of n_1

(ii) Plug n_1 into (W) & solve for n_4

(iii) Plug n_4 into total to calculate n_1

Splitting Mat Balances

W: —

DA: —

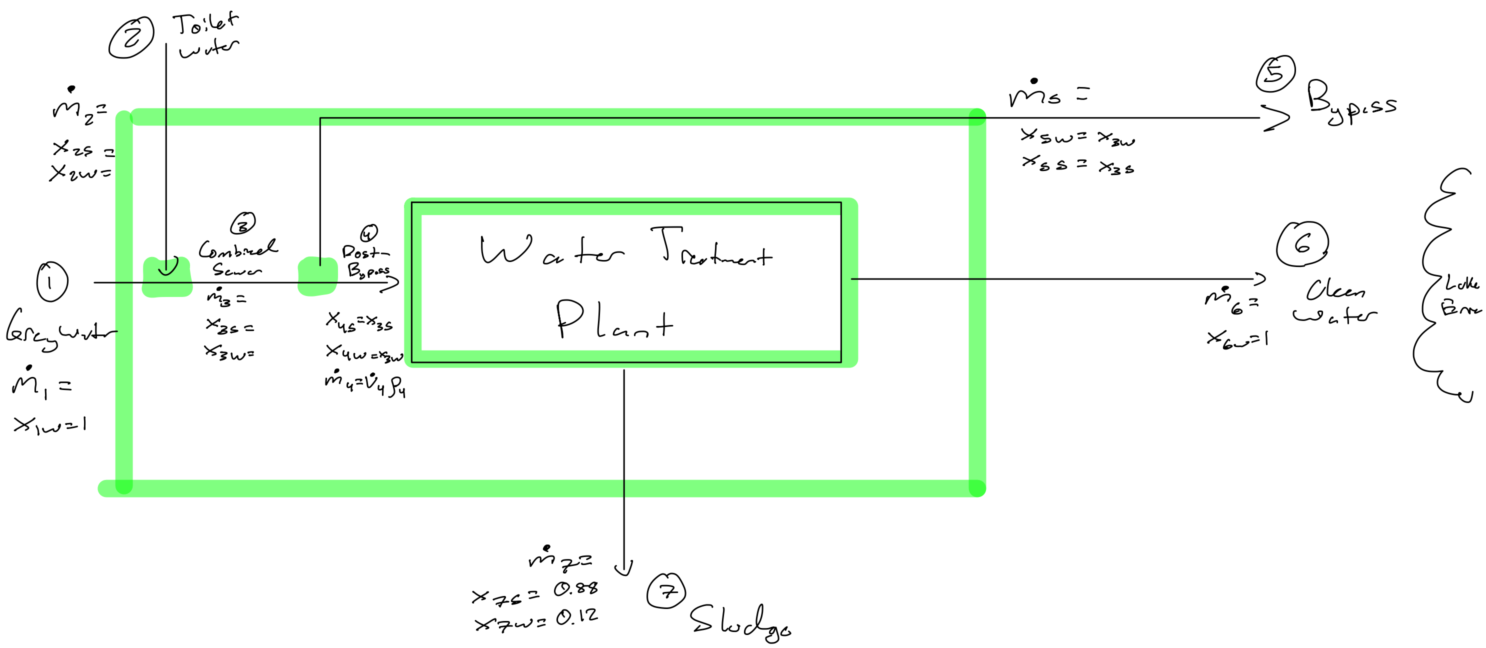
Total: $n_6 = n_3 + n_4$

How to Solve:

(i) Solve (Total) for n_3

Example 5: Combined sewers have Lake Erie down in the dumps. The Easterly Water Treatment Plant in Cleveland, OH treats an average of 100 million gallons of combined sewer water per day and has a maximum capacity of 400 million gallons per day. For the purposes of this exercise, we will model the water treatment plant as a continuous, steady state process. Cleveland's combined sewer systems has two primary sources of water: (1) grey water collected from outdoor sewers (i.e. rain water, water from washing cars, etc.) and (2) toilet water that contains human waste. Grey water is considered pure water. Toilet water can be approximated as a mixture of solids and water. The Easterly Plant intakes the combined sewer stream (mixture of grey water and toilet water) and outputs two streams: (1) treated water that is fed to Lake Erie and (2) sludge which contains mostly solids and some water. When the plant capacity is exceeded (i.e. on very rainy days), some of the combined sewer stream bypasses the Easterly Plant and is fed directly to Lake Erie. On September 7, the combined sewer stream exceeded the Easterly Plant Capacity by 20wt%. The sludge contains 8wt% of the water that was fed to the Easterly Plant. The composition of the sludge is 88wt% solids and the balance is water. The average density of the combined sewer stream is 10 lbs/gallon.

On September 7 (the day of the overflow), how many lbs. of solids were discharged into Lake Erie? What was the volume of clean water discharged into the lake from the water treatment plant (this excludes water in the bypass)?



Additional Info

$\dot{V}_4 = 400$ million gallons/day

$\rho_4 = 10 \frac{lbs}{gal}$ ★ Need to convert units later

- 8% water in stream 4 exits in stream 7

$\dot{m}_7 x_{7w} = 0.08 \dot{m}_4 x_{4w}$ $\quad \cancel{0.08 x_{4w} = x_{7w}}$

Wrote it this way assumes $\dot{m}_4 = \dot{m}_7$

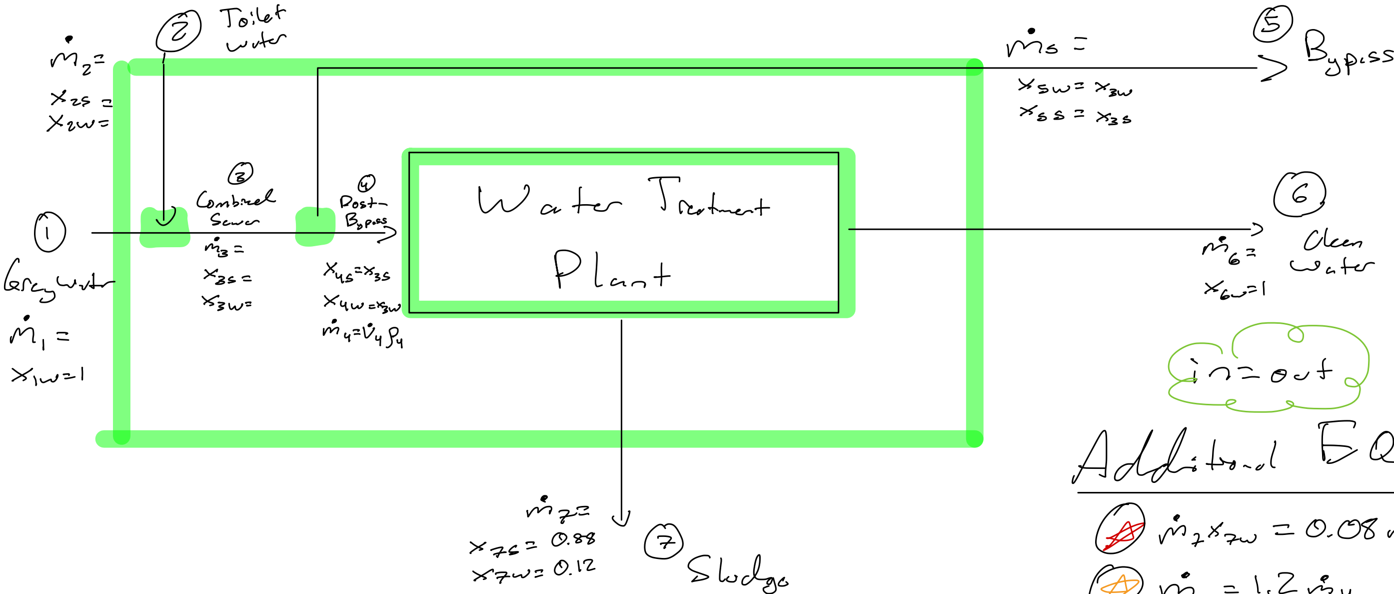
- Combined sewer exceeds capacity by 20 wt%

$\dot{m}_3 = 1.2 \dot{m}_4$ $\quad 0.2 \dot{m}_4 = \dot{m}_5$ ← This is also valid

Want to Know

$\dot{V}_6 = \frac{\dot{m}_6}{\rho_{water}}$

$\dot{m}_5 x_{5s}$



Additional EQs

$\dot{m}_7 x_{7w} = 0.08\, \dot{m}_4 x_{4w}$

$\dot{m}_3 = 1.2\, \dot{m}_4$

$x_{3s} + x_{3w} = 1$

$x_{2s} + x_{2w} = 1$

$x_{5w} + x_{5s} = 1$

Build these into PFD to save time!!

Def. of mass fcts

DoF Analysis

One per subsystem

Water Treatment Plant

4 unknowns ($\dot{m}_6, \dot{m}_7, x_{3w}, x_{3s}$)

−2 indep material balances (b/c 2 species)

−2 additional EQs (⊛, ⊛)

0 DoF solvable

You can find these just here though

Splitting Point

4 unknowns ($\dot{m}_3, x_{3s}, x_{3w}, \dot{m}_5$)

1 indep. material balances (splitting point explained below)

2 additional EQs (⊛, ⊛)

1 DoF ?!

These are all redundant!

S: $\dot{m}_3 \cancel{x_{3s}} = \dot{m}_4 \cancel{x_{4s}} + \dot{m}_5 \cancel{x_{5s}}$

H_2O: $\dot{m}_3 \cancel{x_{3w}} = \dot{m}_4 \cancel{x_{4w}} + \dot{m}_5 \cancel{x_{5w}}$

Total: $\dot{m}_3 = \dot{m}_4 + \dot{m}_5$

Mixing Point

7 Unknowns ($\dot{m}_1, \dot{m}_2, \dot{m}_3, x_{2s}, x_{2w}, x_{3s}, x_{3w}$)

2 indep balances (2 species) ← compositions change @ mixing pt.

2 additional EQs (⊛, ⊛)

3 DoF unsolvable?

Overall

9 Unknowns ($\dot{m}_1, \dot{m}_7, \dot{m}_5, \dot{m}_6, \dot{m}_2, x_{2s}, x_{2w}, x_{5s}, x_{5w}$)

−2 Idep. balances (2 species)

−2 additional EQs (⊛, ⊛)

5 DoF Unsolvable!

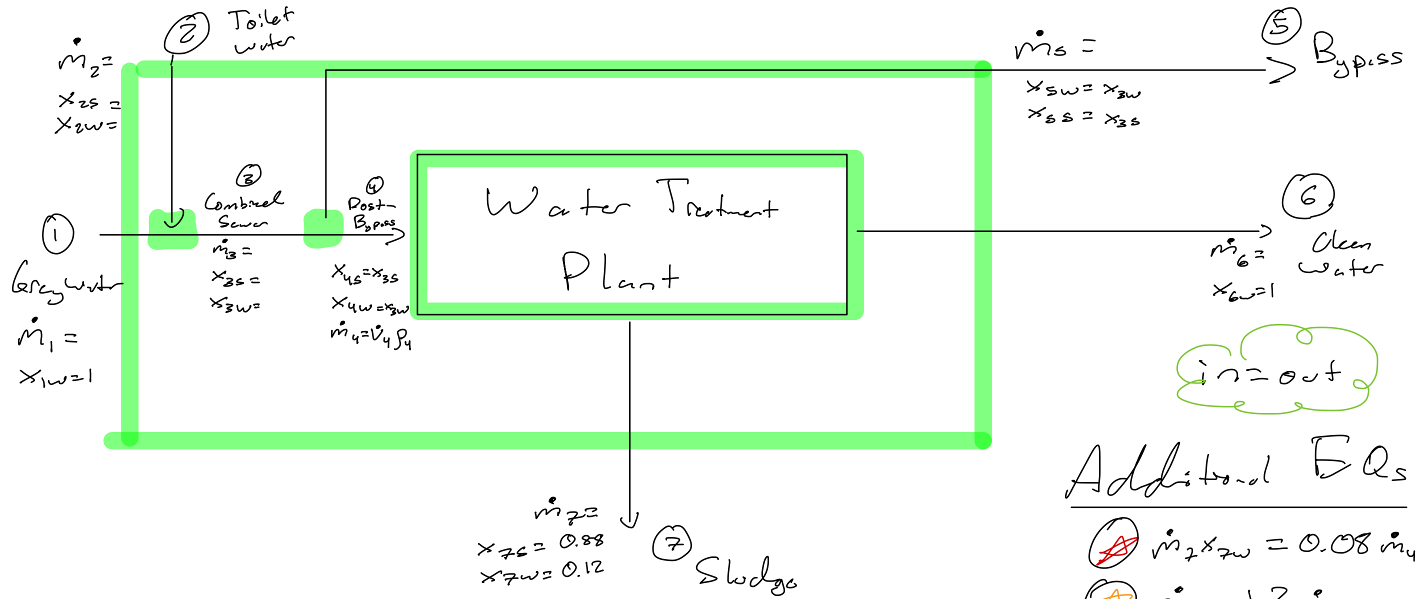
Plan

(i) Solve water Treatment Plant

($\dot{m}_6, \dot{m}_7, x_{3s}, x_{3w}$ will be known)

(ii) Solve Splitting Point to get $\dot{m}_5$

//



Additional EQs

(A) $\dot{m}_7 x_{7w} = 0.08\, \dot{m}_4 x_{4w}$

(B) $\dot{m}_3 = 1.2\, \dot{m}_4$

Material Balances

Treatment

in − out + $\cancel{\text{gen}}^{0}$ − $\cancel{\text{cons}}^{0}$ = $\cancel{\text{accumulation}}^{0}$

in = out

S: $\dot{m}_4 x_{4s} = \dot{m}_7 x_{7s}$

W: $\dot{m}_4 x_{4w} = \dot{m}_7 x_{7w} + \dot{m}_6$

Total: $\dot{m}_4 = \dot{m}_7 + \dot{m}_6$

(A) $\dot{m}_7 x_{7w} = 0.08\, \dot{m}_4 x_{4w}$

$\Rightarrow 0.08\, \dot{m}_4 (1 - x_{4s}) = \dot{m}_7 (1 - x_{7s})$ ☺

Splitting Point

Total:

Solution Strategy

(1) Calculate $\dot{m}_4 = \dot{V}_4$

(2) Solve ☺ for $\dot{m}_7$ and plug into S balance to solve for x_{4s}

(3) Use x_{4s} in S balance to solve for $\dot{m}_7$

(4) Use total to calc $\dot{m}_6$

(5) Calc $x_{4w} = 1 - x_{4s}$

Plan: treatment → splitting

$\boxed{\text{Mat Balance - Treatment}}$ in − out + $\cancel{\text{gen}}^{0}$ − $\cancel{\text{cons}}^{0}$ = $\cancel{\text{accumulation}}^{0}$

no rxns — Cont. steady state

$x_{4w} + x_{4s} = 1$

S: $\dot{m}_4 x_{4s} = \dot{m}_7 x_{7s}$

W: $\dot{m}_4 x_{4w} = \dot{m}_7 x_{7w} + \dot{m}_6$

total: $\dot{m}_4 = \dot{m}_7 + \dot{m}_6$

(*) $0.08\, \dot{m}_4 x_{4w} = \dot{m}_7 x_{7w}$

☺ $0.08\, \dot{m}_4 (1 - x_{4s}) = \dot{m}_7 (1 - x_{7s})$

How to Solve

1. Calculate $\dot{m}_4 = \dot{V}_4 \rho$
2. Solve ☺ for $\dot{m}_7$ and plug into S − solve x_{4s}
3. Use x_{4s} in S balance, solve for $\dot{m}_7$
4. Use total to calc $\dot{m}_6$
5. Calc $x_{4w} = 1 - x_{4s}$

$\boxed{\text{Splitting point}}$

$\dot{m}_3 = \dot{m}_4 + \dot{m}_5$ an $\dot{m}_3 = 1.2\, \dot{m}_4$

6. calculate $\dot{m}_3$ from (**)
7. Calc $\dot{m}_5$ from mat balance

Material Balances on Reactive Systems

Stoichiometry: Remember to balance all chemical reactions!

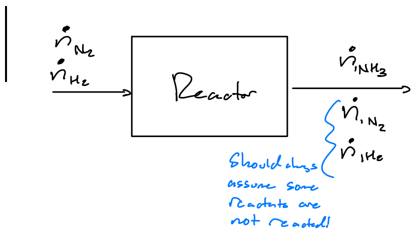
Ex: Haber-Bosch Process combines nitrogen with hydrogen to create ammonia

See WS/ Handout

(i) Write a balanced chemical reaction

(ii) If 100 mol of nitrogen fed to reactor, how many mols ammonia produced?

Consider the chemical reaction for producing ammonia:



$$N_2 + 3H_2 \rightarrow 2NH_3$$

Jargon for chemical reactions

Stoichiometric proportion: Occurs when a ratio of moles present is equal to the ratio of the stoichiometric coefficients in a balanced EQ.

"H_2 and N_2 fed in a stoich proportion"

Additional EQ $\Rightarrow \dfrac{\dot{n}_{N_2}}{\dot{n}_{H_2}} = \dfrac{1}{3}$ could be an additional EQ !!

Limiting reactant: A reactant that is present in less than its stoichiometric proportion relative to every other reactant.

"We feed 3 mol H_2 and 0.5 mol N_2"

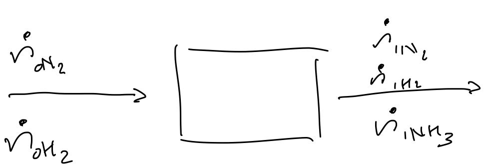
$\Rightarrow N_2$ is the limiting reactant

Excess reactant: A reactant that is present in more than its stoichiometric proportion relative to every other reactant.

$\Rightarrow H_2$ is in excess

Fractional conversion: Ratio of (moles reacted)/(moles fed) for a given reactant.

$\frac{1}{2} NH_3$ only works with a perfect reactor



$$f_i = \frac{\dot{n}_{i,\text{reacted}}}{\dot{n}_{i,\text{fed}}} \qquad f_{N_2} = \frac{\dot{n}_{N_2} - \dot{n}_{1N_2}}{\dot{n}_{N_2}}$$

i = species

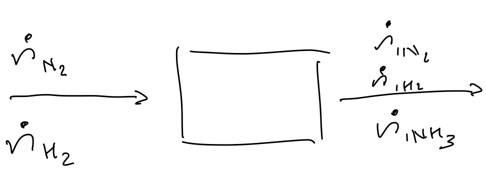
Extent of Reaction (extent of conversion): Indicates how far the reaction proceeds. You can think of this as a combined term that describes the net effect of generation and consumption for a chemical reaction. You can write one for each reaction

in − out + $\underbrace{\text{gen} - \text{cons}}_{}$ = ~~accumulation~~ 0 Batch or Cts. Steady State

Keep for a chemical rxn. described by "extent of rxn"

Extent of Reaction:

ξ = "xi" (lowercase) = Ξ



Out = in + gen/consumption

$$n_{i,1} = n_{i,0} + \sum \nu_{ij} \xi_j$$

ν_{ij} = stoich coef. of species i in rxn j

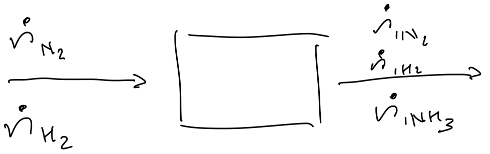
$n_{i,1}$ = moles of i out

$n_{i,0}$ = moles of i in

ξ_j = extent of rxn for reaction j

$+\nu$ = when species is generated

$-\nu$ = when species is consumed



$N_2 + 3H_2 \rightarrow 2NH_3$

$A \rightarrow 3B$

$1 \neq 3$

Moles are not conserved!

For 1 single Rxn ($j=1$)

$$\dot{n}_{i,1} = \dot{n}_{i,0} + \nu_i \dot{\xi}$$

Material Balances (for Haber process)

When working with reactive systems, you must work with moles!!

N_2: $\dot{n}_{N_2,1} = \dot{n}_{N_2,0} + (-1)\xi$ $\quad \nu_{N_2} = 1$ from EQ

Consuming!

H_2: $\dot{n}_{H_2,1} = \dot{n}_{H_2,0} + (-3)\xi$ $\quad \nu_{H_2} = 3$ from EQ

Generating

NH_3: $\dot{n}_{NH_3,1} = 0 + 2\xi$ $\quad \nu_{NH_3} = 2$ from EQ

Total? Moles are not conserved cannot write a total balance for reactive systems!!! No!!