



Unit 1



Unit 1: Units and Process Variables

Process Variables

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

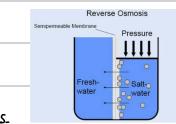
① Salt Water Desalination

Large scale thermal distillation may be energy and cost intensive

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

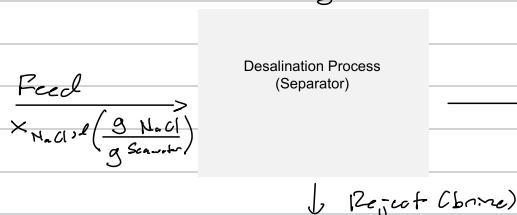
or measured

Tampa Bay Distillation



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

Process Flow Diagram for desalination



↓ Reject Brine)

Flowrate Calculations

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

$$\dot{V} = 25,000,000 \text{ gal/day}$$

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

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

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

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

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

Suppose 100g seawater are present

$$\begin{cases} \rightarrow 3.5 \text{ g NaCl} \times \frac{1 \text{ mol NaCl}}{58.04 \text{ g}} \\ \text{Assume Basis} \end{cases}$$

$$\rightarrow 96.5 \text{ g H}_2\text{O} \times \frac{1 \text{ mol H}_2\text{O}}{18.02 \text{ g}}$$

• Temperature, T

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

Relevant Process Variables

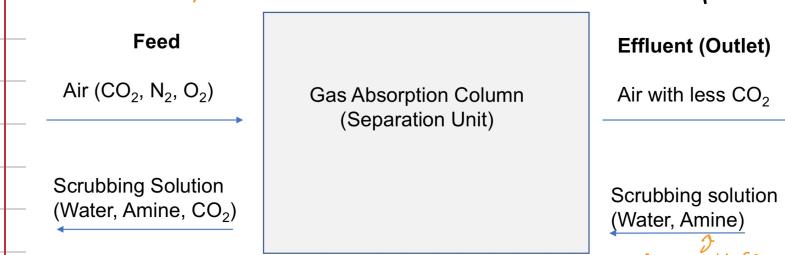
- mass fraction: $\frac{\text{mass of } i}{\text{mass of mixture}} = x_i \text{ or } y_i$ For systems reacting with products
- mol fraction: $\frac{\text{mol of } i}{\text{moles of mixture}} = \bar{x}_i \text{ or } \bar{y}_i$ for gases/vapors

• Pressure, P

- Mass Flowrate, \dot{m} ($\frac{\text{mass}}{\text{time}}$)
- Volumetric Flowrate, \dot{V} ($\frac{\text{volume}}{\text{time}}$)
- Molar Flowrate, \dot{n} ($\frac{\text{moles}}{\text{time}}$)
- Energy Flowrate, \dot{H} ($\frac{\text{energy}}{\text{time}}$)

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



Assume our behaviors ideally and consider that absorption with $n_i = 1 \text{ mol/min}$.

Write an equation for V_i :

$$PV = n_i RT \quad \text{and} \quad P_i V_i = n_i R T \quad \text{is also valid}$$

Be specific about stream which is ideal

$$\rightarrow V_i = \frac{n_i R T}{P_i}$$

Consider air is a mixture of CO_2 , N_2 , O_2 . By mass: 76.95% N_2 , 0.05% CO_2 , and 23% O_2 .

Weighted Average Properties of a mixture: $MW_{\text{air}} (\text{g/mol}) = \sum y_i MW_i$

where y_i = molar masses of all species i
 x_i = mole fractions of all species i

$$\therefore MW_{\text{air}} (\text{g/mol}) = y_{\text{N}_2} MW_{\text{N}_2} + y_{\text{CO}_2} MW_{\text{CO}_2} + y_{\text{O}_2} MW_{\text{O}_2}$$

Process for Solving

- Look up all MW
 - Convert mass fraction to mol fraction for all species
- Assume a basis for gas calculations, 100 g air

Relevant Process Variables

- Air Pressure
 - Amine: CO_2 Reactions
 - ↳ Solution Concentrations
 - Fraction CO_2 Removed
 - Flowsheet (x_i, y_i, v_i, F_i) $i = \text{species}$
 - ↳ Total Flowsheet (x_i, y_i, v_i) gases
 - Composition of each stream (x_i vs. y_i)
 - Energy Flowsheets (H_i)
 - Temperature and Pressure
- Indirect Discussion
- Group Discussion

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'
Example: Beverage fermentation, Pharmaceutical, and Food Productions
- Continuous:** Reactants and Products continuously flow in and out of the reactor
Example: 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
Example: Polymerization reactions, Exothermic Reactions (Diluting Reactions)

Steady-State vs. Transient Processes

- we do
thus type:
thus 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: $\text{in} - \text{out} + \text{accumulation} - \text{consumption} = 0$

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

1. Draw and label a process flow diagram (PFD)



Material R
use mostly

- Label All streams with Known process variables (T_i, P_i, x_i, y_i)
- Label All streams with Unknown 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 system
- # additional mathematical relationships

DOF

If $DOF \leq 0$, then... *solve!*

If $DOF > 0$, then... *Cannot solve...* This is an unsolvable answer

3. Convert all quantities to the same basis

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

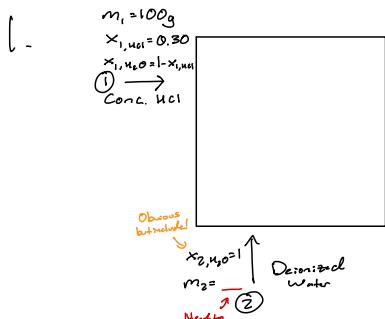
5. Write all material balances for all necessary subsystems

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

Example 1: Diluting HCl. 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?



2. Degree of Freedom (DOF) Analysis

Derived from law of cons. of mass: \rightarrow 1 unknown (mass) \rightarrow 1 independent material balance \rightarrow 1 additional eqns. \rightarrow 0 additional eqns.

Can write 2 more as there are 2 species ($\text{HCl} + \text{H}_2\text{O}$)

in-out of gen-cons. = accumulation

Mass # species! \rightarrow 2 unknowns \rightarrow 2 material balances \rightarrow 0 additional eqns.

$$2 - 2 - 0 = 0 \text{ DOF } \textcircled{4}$$

3. All Process Variables on same basis?
Are we dimensionally consistent? ✓

4. Material Balances

in - out + generation - consumption = accumulation
(gen) (cons)

No chemical reaction

Every thing counts
we have a batch process!

$$\rightarrow \text{in} - \text{out} = 0 \quad \text{so} \quad \text{in} = \text{out}$$

5. $\text{HCl} : m_1 x_{1,\text{HCl}} = m_3 x_{3,\text{HCl}}$

$\text{H}_2\text{O} : m_1 x_{1,\text{H}_2\text{O}} + m_2 x_{2,\text{H}_2\text{O}} = m_3 x_{3,\text{H}_2\text{O}}$

Add up inip and \rightarrow Total Mass: $m_1 + m_2 = m_3$

cancel out with mass fractions

$$m_1 x_{1,\text{HCl}} + m_1 x_{1,\text{H}_2\text{O}} + m_2 x_{2,\text{H}_2\text{O}} =$$

$$m_2 x_{3,\text{H}_2\text{O}} + m_3 x_{3,\text{HCl}}$$

$$\rightarrow m_1 (x_{1,\text{HCl}} + x_{1,\text{H}_2\text{O}}) + m_2 (x_{2,\text{H}_2\text{O}} + x_{3,\text{H}_2\text{O}}) =$$

$$m_3 (x_{3,\text{H}_2\text{O}} + x_{3,\text{HCl}})$$

$$\rightarrow m_1 + m_2 = m_3$$

6. Plan of Attack (PoA)

- Solve HCl for m_3
 - Solve H_2O for m_2 using (i) result
- ↳ For ease, solve m_2 from mass balance

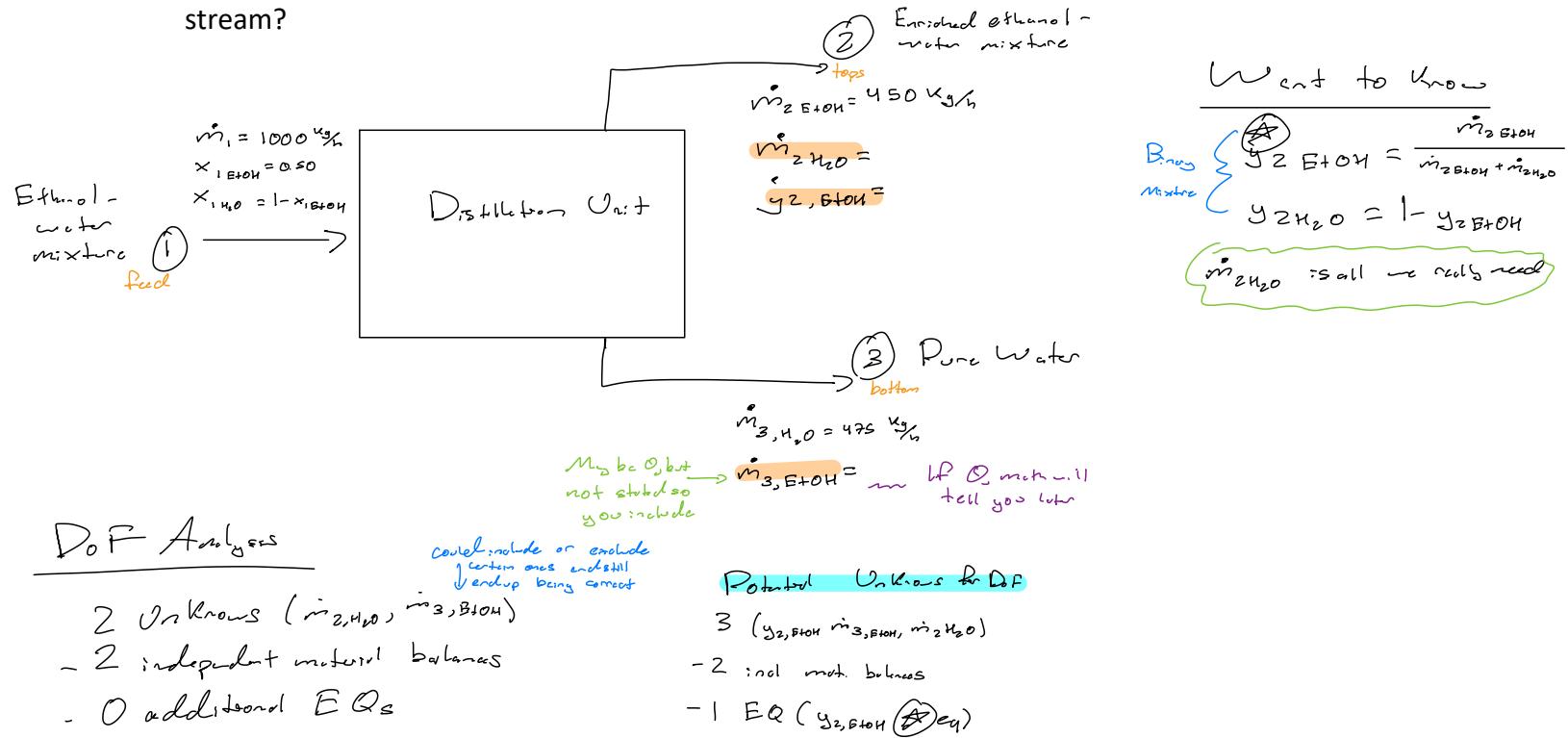
$$7. m_3 = \frac{m_1 x_{1,\text{HCl}}}{x_{1,\text{HCl}}}$$

$$m_1 + m_2 = \frac{m_1 x_{1,\text{HCl}}}{x_{1,\text{HCl}}}$$

$$\rightarrow m_2 = \frac{m_1 x_{1,\text{HCl}}}{x_{1,\text{HCl}}} - m_1$$

Usually stop here or carry

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. What is the composition (by mass) of the top stream?



O Dof $y_{2, \text{EtOH}}$! Its Soluble!

Material Balances

$$\text{in} - \text{out} + \text{generation} - \text{consumption} = \text{accumulation}$$

No physical separation/reaction occurs

$$\rightarrow \text{in} = \text{out}$$

$$\text{EtOH: } m_1, x_{1, \text{EtOH}} = m_{2, \text{EtOH}} + m_{3, \text{EtOH}}$$

$m_1, x_{1, \text{EtOH}} = m_{2, \text{EtOH}} + m_{3, \text{EtOH}}$

$$\text{H}_2\text{O: } m_1, x_{1, \text{H}_2\text{O}} = m_{2, \text{H}_2\text{O}} + m_{3, \text{H}_2\text{O}}$$

$$\text{Total: } m_1 = m_{2, \text{EtOH}} + m_{2, \text{H}_2\text{O}} + m_{3, \text{EtOH}} + m_{3, \text{H}_2\text{O}}$$

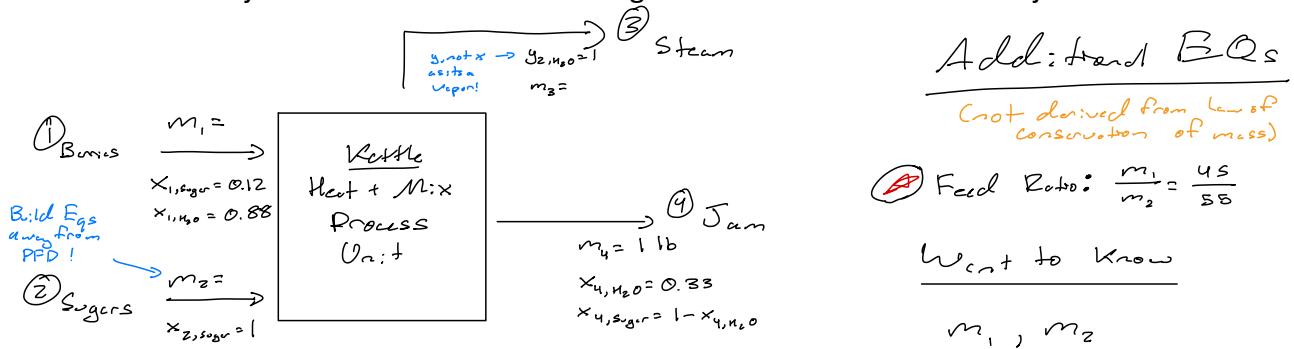
Law of conservation of mass
It's steady-state!
So there is O accumulation

Plan of Attack

(i) Solve H_2O for $m_{2, \text{H}_2\text{O}}$

(ii) Use $m_{2, \text{H}_2\text{O}}$ in ~~eq~~

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?



DOF Analysis

- 3 unknowns (m_1, m_2, m_3)
- 2 independent material balances (two species, sugar & water)
- 1 additional equation (④)

① $\rightarrow \text{DOF} \leq 0 \checkmark$
Can solve!

Material Balances

Always start with law of conservation of mass!
in-out + gen = consumption + accumulation
 $\rightarrow m_i = \text{out}$

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

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

Total: $m_1 + m_2 = m_3 + m_4$

Batch process as final quantity is a mass, not flow rate

Independent Balances

Feed Ratio: $\frac{m_1}{m_2} = \frac{4S}{SS}$

To highlight everything you know

How to Solve

- Solve ④ for m_3
- Plug ④ into sugar balance to solve for m_2
- Plug m_2 into ④ to solve m_1

Solve \checkmark Not needed on HW unless specified

$$(i) m_3 = \frac{4S}{SS} m_2$$

$$(ii) \frac{4S}{SS} m_2 x_{1,sugar} + m_2 = m_4 x_{4,sugar}$$

$$m_2 \left(\frac{4S}{SS} x_{1,sugar} + 1 \right) = m_4 x_{4,sugar}$$

$$m_2 = \frac{m_4 x_{4,sugar}}{\frac{4S}{SS} x_{1,sugar} + 1}$$

(iii) ...

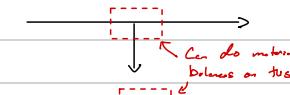
Don't need to do the algebra

Ron LOS

Multi-Unit Processes w/ Recycle and Bypass Streams

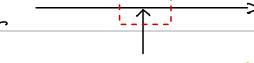
New Terminology

Splitting Point: Where 1 stream becomes 2 streams



Note
Red box is a subsystem
for all pictures
and PFD here

Mixing Point: Where 2 or more streams become 1 Stream



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



Recycle vs. Bypass

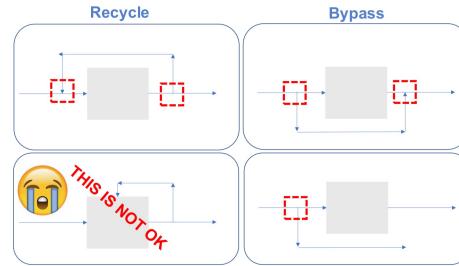
Recycle: Dilute a stream

Circulate a working fluid

Recover a catalyst

Reuse unreacted components

Bypass: Circumvent a unit operation
Overflow condition for safety

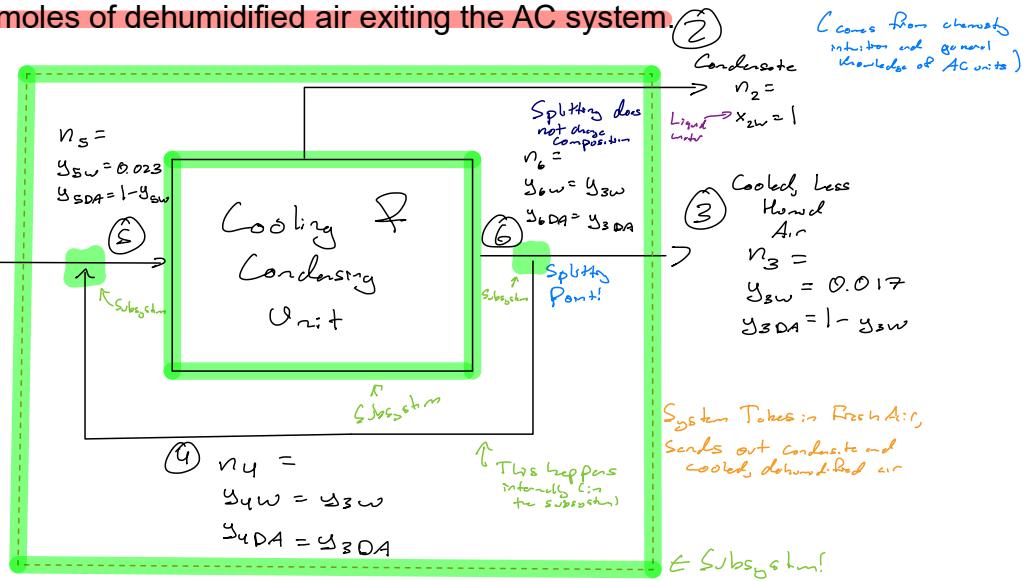


"The stream is
recycled into the
reactor" means stream
going into reactor!
recycled into feed

RECYCLE AND BYPASS (SINGLE AND MULTI UNIT)

Example 4: Air conditioning. An air conditioning system takes in fresh air (4 mol% 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 2.3 mol% 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.

D.F for total
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 constraint ✓

DoF Analysis: *Can do 1 per subsystem present • Entire System, Splitting Point, mixing Point, cooling/condensing*

Overall-DoF: 3 unknowns (n_1, n_2, n_3)

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

- 2 indep. material balances (W, DA)

- 0 additional Eqs *From Curr or the PPD*

Cannot be derived

1 DoF, cannot solve here!

Mixing-DoF: 3 unknowns (n_1, n_2, n_3)

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

- 2 indep. material balances (W, DA)

- 0 additional Eqs *Common one we would be like a mixing ratio*

1 DoF ↴

Cooling/Condensing-DoF: 3 unknowns (n_2, n_3, n_6)

- 2 indep. material balances (W, DA)

0 additional Equations

1 DoF ↴

Only can do it when only compositions are given!

Plan: We have to assume a basis,

look at substreams with DoF's

To avoid assuming basis for what you're looking to find

(i) Go for n_s , as it allows us to solve 2 substreams
 $n_s = 100 \text{ mol}$

(ii) Solve cooling/condensing → mixing

(iii) Use splitting to solve for n_3

Material Balances

highlight as things are known

Cooling / Condensing Mat Balances

$$w: n_3 y_{3,w} = n_6 y_{6,w} + n_2$$

$$DA: n_3 y_{3,DA} = n_6 y_{6,DA}$$

$$\text{Total: } n_3 = n_6 + n_2$$

How to Solve:

- (i) Solve (DA) for n_6
- (ii) Solve (Total) for n_2

Mixing Mat Balances

$$w: n_1 y_{1,w} + n_4 y_{4,w} = n_3 y_{3,w}$$

$$DA: n_1 y_{1,DA} + n_4 y_{4,DA} = n_3 y_{3,DA}$$

$$\text{Total: } n_1 + n_4 = n_3$$

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_3

Splitting Mat Balances

$$w: \quad \quad \quad$$

$$DA: \quad \quad \quad$$

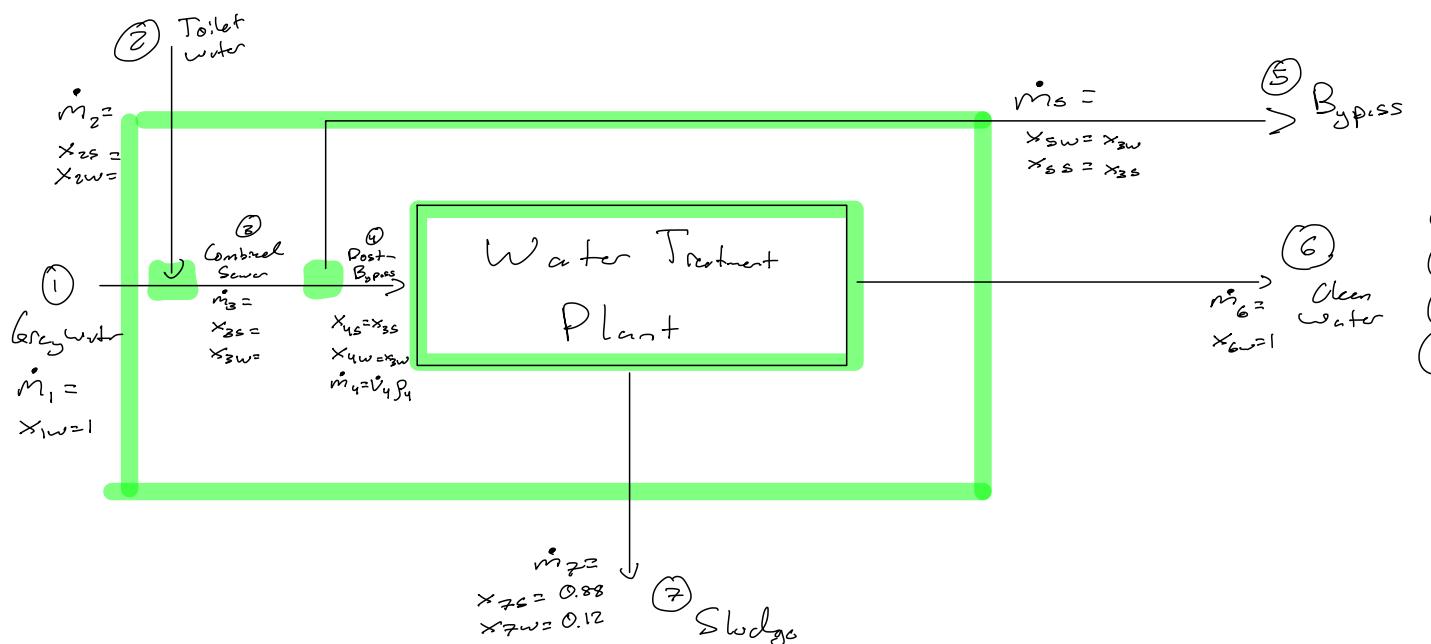
$$\text{Total: } n_6 = n_3 + n_4$$

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

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

$$\rho_4 = 10 \frac{\text{lbs}}{\text{gallon}}$$

* Needs to convert units later

- 8% water in stream 4 exists in stream 7

$$\dot{m}_2 x_{2w} = 0.08 \dot{m}_4 x_{4w} \quad \text{(0.08} x_{4w} = x_{2w})$$

- Combined sewer exceeds capacity by 20 wt%

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

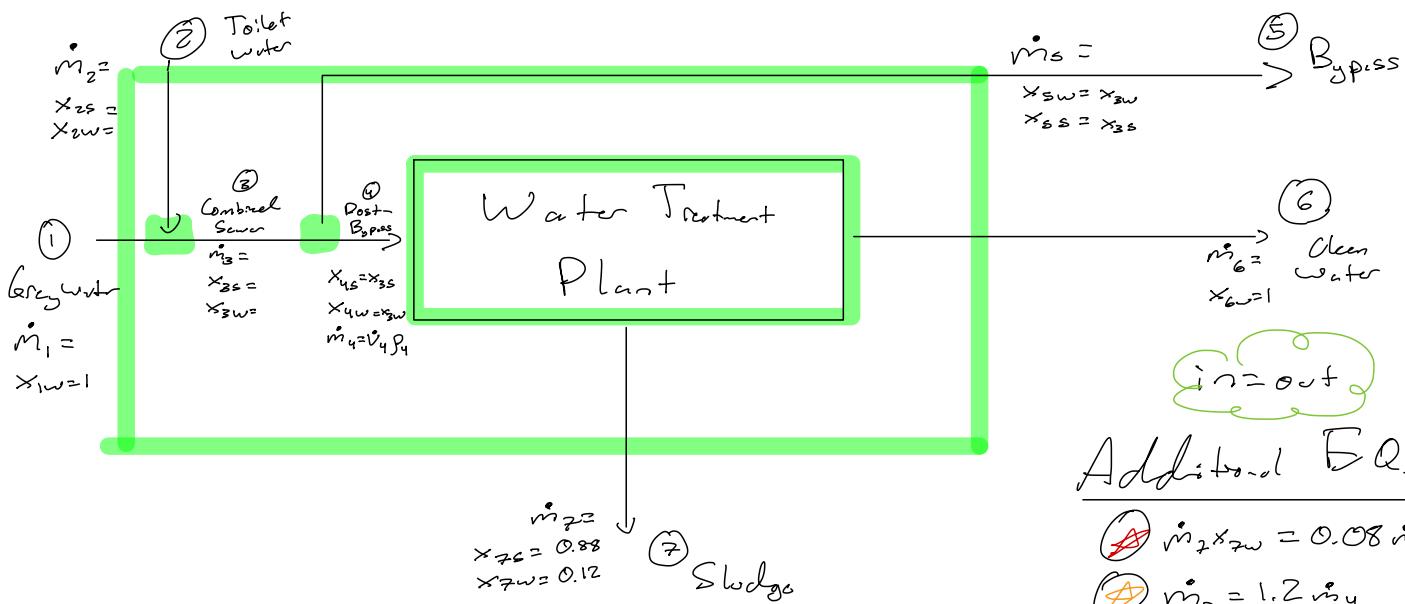
$$0.2 \dot{m}_4 = \dot{m}_5 \quad \text{This is also valid}$$

Want to know

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

$$\dot{m}_5 x_{ss}$$

Wants to know
way assumes
 $\dot{m}_4 = \dot{m}_7$



DoF Analysis One per subsystem

Water Treatment Plant

- You can pinhole just here
down
- 4 unknowns (m_5 , m_7 , x_{3w} , x_{8s})
 - 2 indep. material balances (b/c 2 species)
 - 2 add. transl. Eqs (del $\textcircled{1}$, del $\textcircled{2}$)
- 0 DoF Solvent

(Splitting Point)

- 4 unknowns (m_3 , x_{2s} , x_{3w} , m_6)
- 1 indep. material balance (Splitting point explained below)
- 2 additional Eqs (del $\textcircled{1}$, del $\textcircled{2}$)

1 DoF $\frac{1}{1}$

Si: $m_3 x_{2s} = m_4 x_{2s} + m_5 x_{2s}$

H₂O: $m_3 x_{2w} = m_4 x_{2w} + m_5 x_{2w}$

Toatl: $m_3 = m_4 + m_5$

This one already

Mixing Point

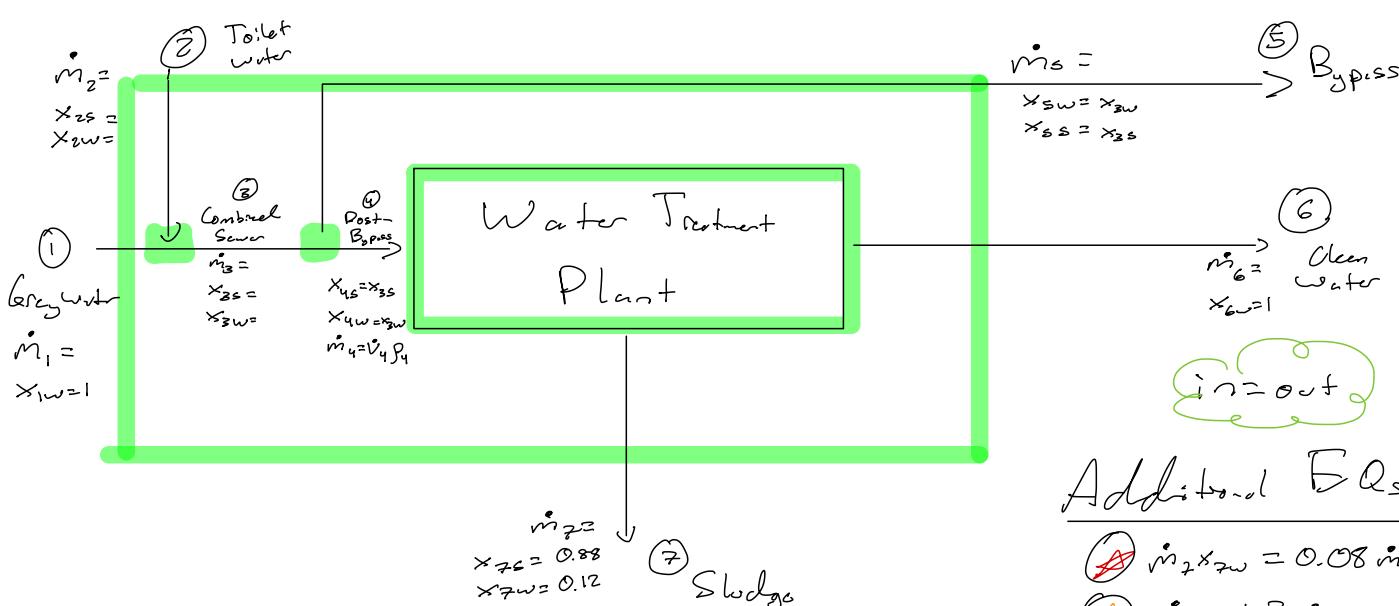
- 7 unknowns (m_1 , m_2 , m_3 , x_{2s} , x_{2w} , x_{3s} , x_{3w})
- 2 indep. balances (2 species) ← composition chose @ mixing pt.
- 2 additional Eqs (del $\textcircled{1}$, del $\textcircled{2}$)
- 3 DoF unsolvable!

Overall

- 9 unknowns (m_1 , m_2 , m_3 , m_4 , m_5 , x_{2s} , x_{2w} , x_{3s} , x_{3w})
- 2 indep. balances (2 species)
- 2 additional Eqs (del $\textcircled{1}$, del $\textcircled{2}$)
- 5 DoF Unsolvble!

Plan

- (i) Sole water Treatment Plant
(m_6 , m_7 , x_{3s} , x_{3w} will be known)
- (ii) Sole Splitting Point to get m_3



Material Balances

Treatment

$$\text{in-out + gen-cons} = \text{accumulation}$$

$$\text{in-out}$$

$$S: m_4 x_{4s} = m_7 x_{7s}$$

$$W: m_4 x_{4w} = m_7 x_{7w} + m_6$$

$$\text{Total: } m_4 = m_7 + m_6$$

~~$$m_2 x_{3w} = 0.08 m_4 x_{4w}$$~~

$$\Rightarrow 0.08 m_4 (1 - x_{4s}) = m_2 (1 - x_{3s}) \quad (y)$$

Splitting Point

See SS on Right

Plan: treatment \rightarrow splitting

MAT Balance - Treatment	in-out+gen-cons=accumulation
S: $m_4 x_{4s} = m_7 x_{7s}$	norms $x_{4w} + x_{4s} = 1$
W: $m_4 x_{4w} = m_7 x_{7w} + m_6$	Cont. Steady state $0.08 m_4 x_{4w} = m_7 x_{7w}$
total: $m_4 = m_7 + m_6$	(z) $0.08 m_4 (1 - x_{4s}) = m_2 (1 - x_{3s})$

How to Solve

$$1. \text{ Calculate } m_4 = \dot{V}_4 \rho_4$$

$$2. \text{ Solve } (y) \text{ for } m_7 \text{ and plug into } S - \text{solve } x_{4s}$$

$$3. \text{ Use } x_{4s} \text{ in } S \text{ balance, solve for } m_7$$

$$4. \text{ Use total to calc } m_6$$

$$5. \text{ calc } x_{4w} = 1 - x_{4s}$$

Splitting Point

$$m_3 = m_4 + m_5 \quad \text{and} \quad m_3 = 1.2 m_4$$

$$6. \text{ calculate } m_5 \text{ from } (y)$$

$$7. \text{ calc } m_5 \text{ from mat balance}$$

Now we have m_6 and $m_5 x_{5s}$
because $x_{3s} = x_{5s}$.

Solution Steps

$$(1) \text{ Calculate } m_4 = \dot{V}_4$$

$$(2) \text{ Solve } (y) \text{ for } m_7 \text{ and plug into } S \text{ balance to solve for } x_{4s}$$

$$(3) \text{ Use } x_{4s} \text{ in } S \text{ balance to solve for } m_7$$

$$(4) \text{ Use total to calc } m_6$$

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

Material Balances on Reactive Systems

Stoichiometry: Remember to balance all chemical reactions!

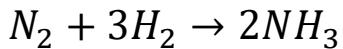
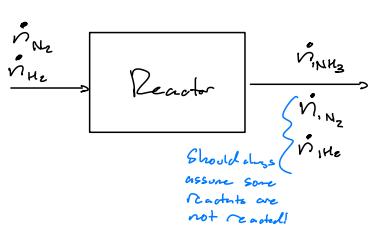
Ex: Haber-Bosch Process combines nitrogen with hydrogen to create ammonia.

See WS/
Handout

(i) Write a balanced chemical reaction
(ii) If 100 mol of nitrogen fed to reactor, how many mols ammonia produced?

Unit 3: Material Balances on Reactive Systems

Consider the chemical reaction for producing ammonia:



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 propn."

$$\Rightarrow \frac{\dot{v}_{N_2}}{\dot{v}_{H_2}} = \frac{1}{3}$$

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 "

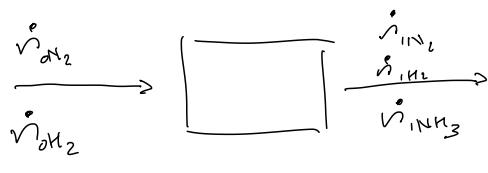
$\Rightarrow N_2$ is the limiting reactant

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

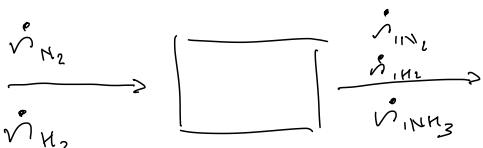


$$f_i = \frac{\dot{v}_{i, \text{reacted}}}{\dot{v}_{i, \text{fed}}}$$

$i = \text{species}$

$$f_{N_2} = \frac{\dot{v}_{N_2} - \dot{v}_{H_2}}{\dot{v}_{N_2}}$$

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*



$$\text{in-out + gen-consum} = \text{accumulation}$$

Batch or Cts. steady state

Keep in mind: chemical rxn. described by "ext of rxn"

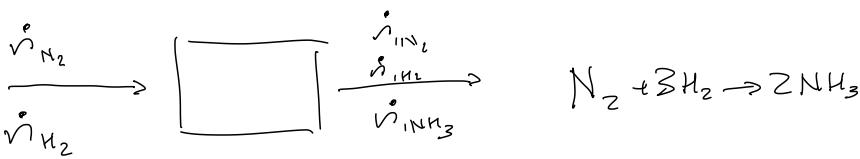
$$\text{Out} = \text{in} + \text{gen/consum}$$

$$n_{i,i} = n_{i,0} + \sum \gamma_{ij} \bar{z}_j$$

Extent of Reaction:

$$\bar{z} = \frac{n_{i,i}}{n_{i,0}} = \frac{\text{out}}{\text{in}}$$

γ_{ij} = stoich. coef. of species i in rxn j
 $n_{i,i}$ = moles of i out
 $n_{i,0}$ = moles of i in
 \bar{z}_j = extent of rxn for reaction j
+ \bar{z} = when species is generated
- \bar{z} = when species is consumed



For single R_m ($j=1$)

$$\dot{n}_{i,s} = \dot{n}_{i,0} + \dot{v}_i \bar{z}$$

Material Balances (for Haber process)

$$N_2: \dot{n}_{N_2} = \dot{n}_{N_2,0} + (-1)\bar{z} \quad \bar{z}_{N_2} = 1 \text{ from EO}$$

$$H_2: \dot{n}_{H_2} = \dot{n}_{H_2,0} + (3)\bar{z} \quad \text{Consuming!} \quad \bar{z}_{H_2} = 3 \text{ from EO}$$

$$NH_3: \dot{n}_{NH_3} = 0 + 2\bar{z} \quad \text{Generating!} \quad \bar{z}_{NH_3} = 2 \text{ from EO}$$

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

$A \rightarrow 3B$

$\neq 3$

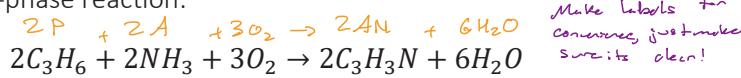
Moles are not conserved!

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

Unit 5: Material Balances on Reactive Systems

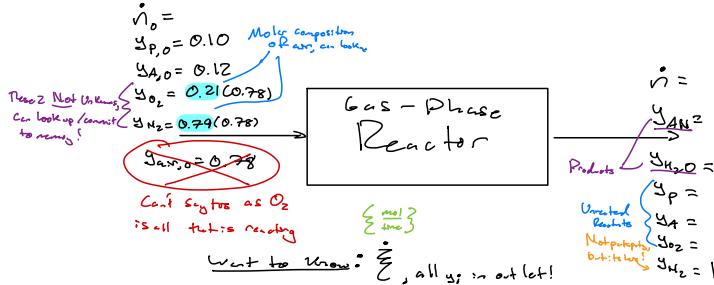
Example 1: Production of acrylonitrile

Acrylonitrile is an important precursor for many consumer goods! Synthesis of acrylonitrile proceeds according to the following gas-phase reaction:



The feed to the reactor contains 10 mol% propylene (C_3H_6), 12 mol% ammonia (NH_3) and 78 mol% air. The process has a 30% conversion of the limiting reactant. What are the limiting and excess reactants? What is the extent of reaction? What is the composition of the product stream?

PPD



Addl. Reactn Eqs

$$f_p = \frac{\text{mol P reacted}}{\text{mol P fed}} = \frac{n_{P\text{out}} - n_{P\text{in}}}{n_{P\text{in}}} = 0.30$$

Alternate Approach

$$\begin{aligned} n_{AN} &= \\ n_{H_2O} &= \\ n_P &= \\ n_A &= \\ n_{O_2} &= \\ n_{N_2} &= \end{aligned}$$

DoF Analysis

Reactn: Assume $n_0 = 100 \text{ mol}$
 6 Unknowns (n_{O_2} is 5 y_i from outlet stream)
 - 6 Indep. Mat. Balances (bc 6 species: AN, H_2O , P , A , O_2 , N_2)
 - 1 Additional Eq (fp)
 +1 Chemical Reaction ($\frac{2}{3}$) \leftarrow Extent of Reaction is added to DoF!

∂X DoF $\approx \leftarrow$ Assume a Basis to bring DoF to 0.

Material Balances

Note: $2P + 2A + 3O_2 \rightarrow 2AN + 6H_2O$

in-out-gain-loss = accumulation

$$G_{\text{in}} \rightarrow n_i = n_{i,0} + \dot{n}_i \frac{t}{2}$$

$$P: n_{y_P} = n_0 y_{P,0} + (-2) \frac{t}{2}$$

$$A: n_{y_A} = n_0 y_{A,0} + (-2) \frac{t}{2}$$

$$N_2: n_{y_{N_2}} = n_0 y_{N_2,0} + 0 \frac{t}{2}$$

No Reactive Species (Inert)
Results in: in = out

$$t_2 O_2: n_{y_{H_2O}} = 0 + 6 \frac{t}{2}$$

$$AN: n_{y_{AN}} = 0 + 2 \frac{t}{2}$$

$$O_2: n_{y_{O_2}} = n_0 y_{O_2,0} + (-3) \frac{t}{2}$$

Cannot write a total balance as moles are not a conserved quantity!!!

How to Solve

(i) Solve f_p for n_{y_P} \rightarrow Plug into P balance \rightarrow solve $\frac{t}{2}$

(ii) Solve A balance for n_{y_A} ($\frac{\text{moles } A}{t}$)

(iii) Solve N_2 balance for $n_{y_{N_2}}$

(iv) Solve H_2O balance for $n_{y_{H_2O}}$

(v) Solve AN for $n_{y_{AN}}$

(vi) Solve O_2 for $n_{y_{O_2}}$

(vii) Calculate n_{y_P} from f_p

(viii) Calculate mol fraction of each species in outlet stream

$$y_i = \frac{n_i}{\sum n_i} = \frac{\text{moles of } i}{\text{total moles}} \quad \leftarrow \text{Given generic definition in terms of what you solved for}$$

Addl. Reactn Eqs

$$f_p = \frac{\text{mol P reacted}}{\text{mol P fed}} = \frac{n_{P\text{out}} - n_{P\text{in}}}{n_{P\text{in}}} = 0.30$$