CHEMICAL PROCESS CALCULATIONS

(Introduction to engineering calculations)

Lecture #2: August 07, 2023

Introduction

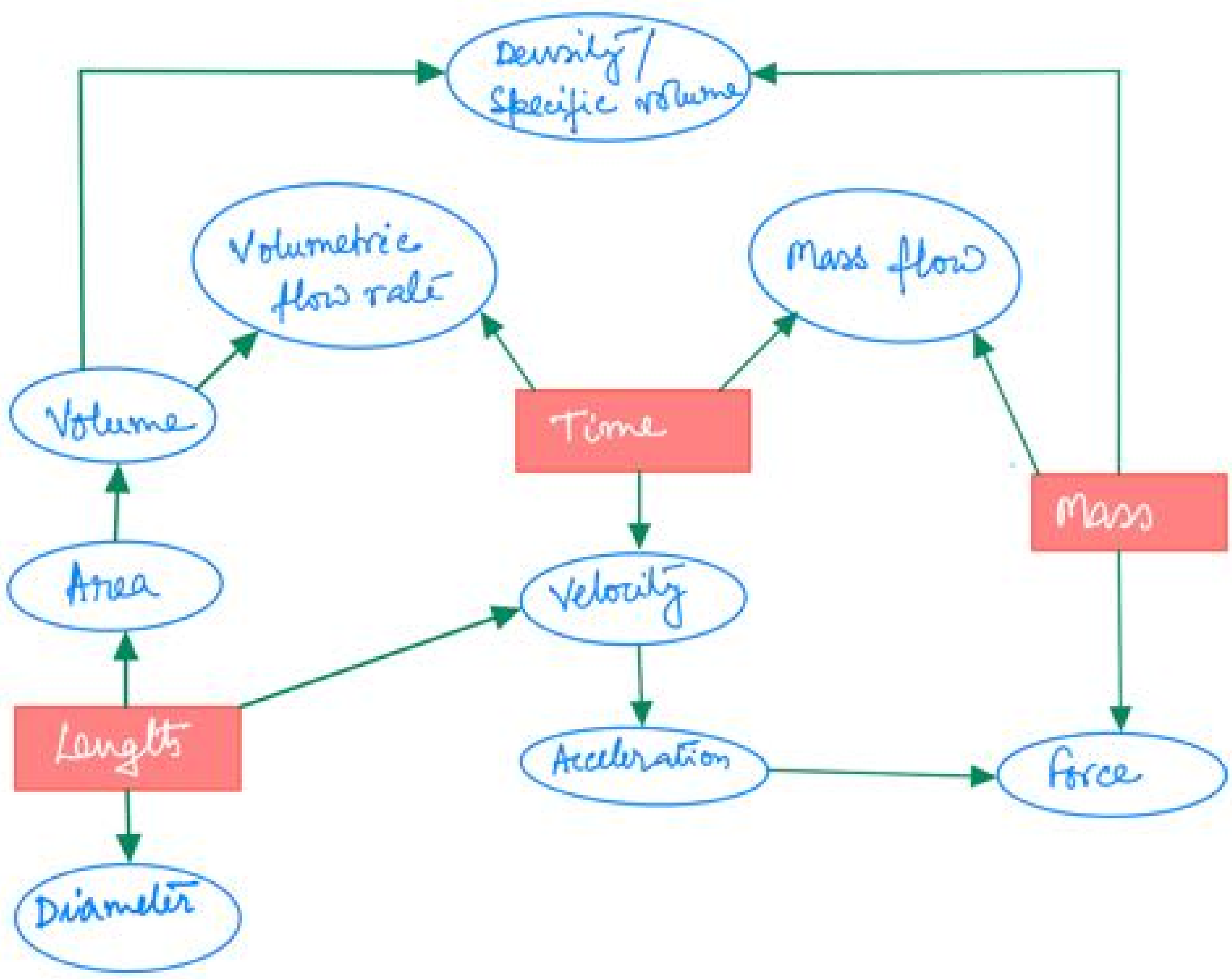
- Dealing with processes that are designed to convert raw materials into desired products

- Dimensions, units, and their conversion
- Processes and process variables
- Material balances
- Energy balances

Dimensions & Units

- Dimension – a measurable property
  - Basic (length, time, mass, temperature, molar amount)
  - Derived (velocity, density, pressure, flow rate, etc.)
- Unit – means of expressing dimensions
  - m – length, s – time, g – mass, K – temperature
  - Base units
  - Multiple units
  - Derived units

Basic and derived dimensions



Basic and derived dimensions

Basic		
Dimension	Unit	Symbol
Length	meter	m
Mass	kilogram	kg
Moles	gram-mole	mol or g-mole
Time	second	s
Temperature	kelvin	K
Electric current	ampere	A
Light intensity	candela	cd

Derived Units			
Dimension	Unit	Symbol	Equivalent
Volume	liter	L	$0.001\ m^3$
Force	newton	N	$1\ kg\ m/s^2$
Pressure	pascal	Pa	$1\ N/m^2$
Energy	joule	J	1 N m
Power	watt	W	1 J/s

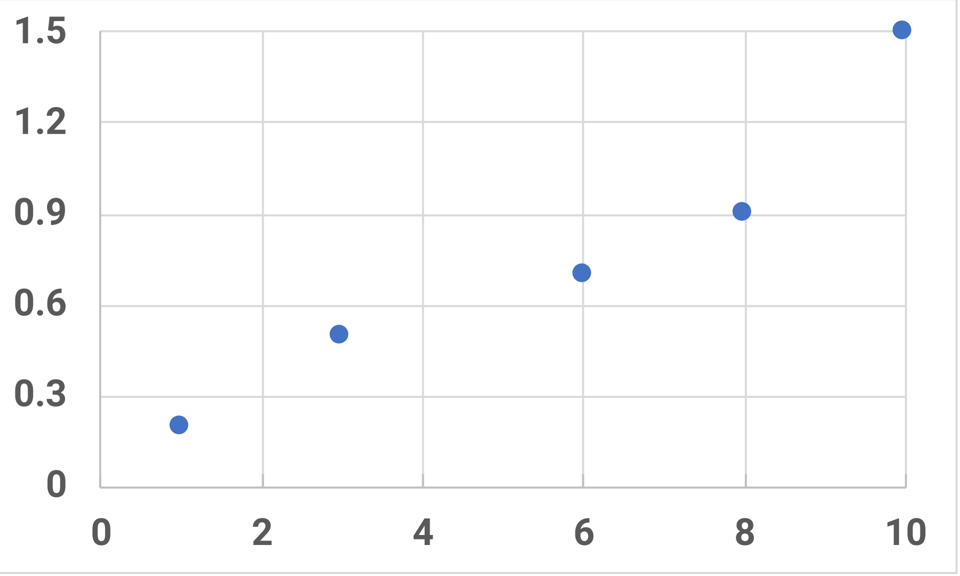
Multiple Unit	
tera (T) = 10^{12}	nano (n) = 10^{-9}
giga (G) = 10^{9}	micro (μ) = 10^{-6}
mega (M) = 10^{6}	milli (m) = 10^{-3}
kilo (k) = 10^{3}	centi (c) = 10^{-2}

Dimensional homogeneity

- Valid equation must be dimensionally homogeneous
  - u_2 (m/s) = u_1 (m/s) + g (m/s^2) t (s)
  - homogeneous and consistent
- Dimensionally homogeneous equation may not necessarily be always valid
- D (m) = 55 t (min) + 1.22
- Dimensionless quantity

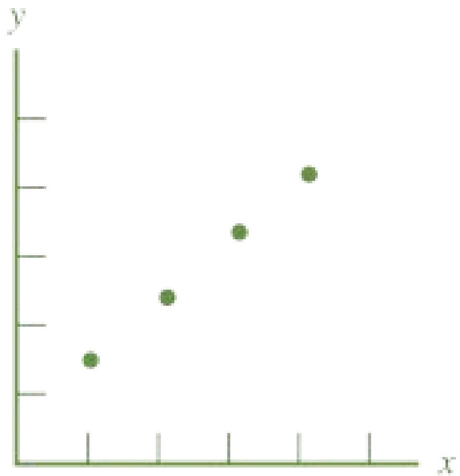
Data representation & analysis

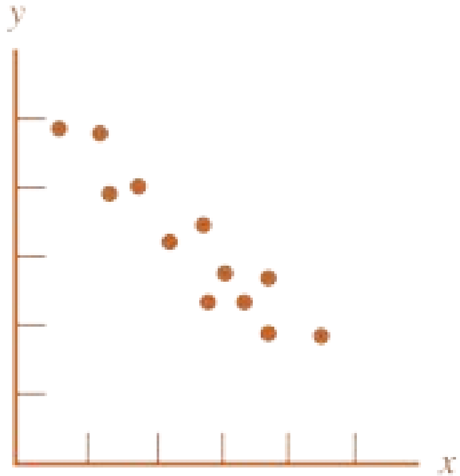
x	1	3	6	8	10
y	0.2	0.5	0.7	0.9	1.5

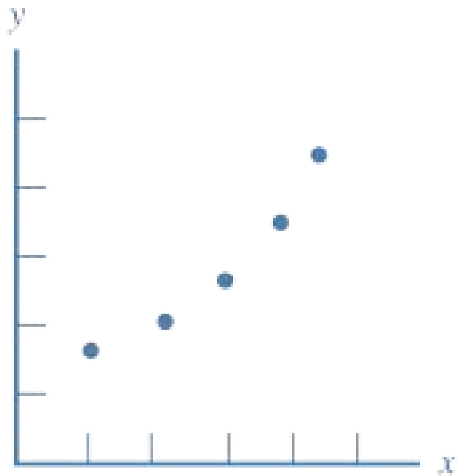


interpolation / extrapolation

Data representation & analysis







$$y = y_1 + \frac{x - x_1}{x_2 - x_1}(y_2 - y_1)$$

Two-point linear interpolation

Data representation & analysis

$y = 5x + 4$

$y = 5(x-2)^2 - 25$

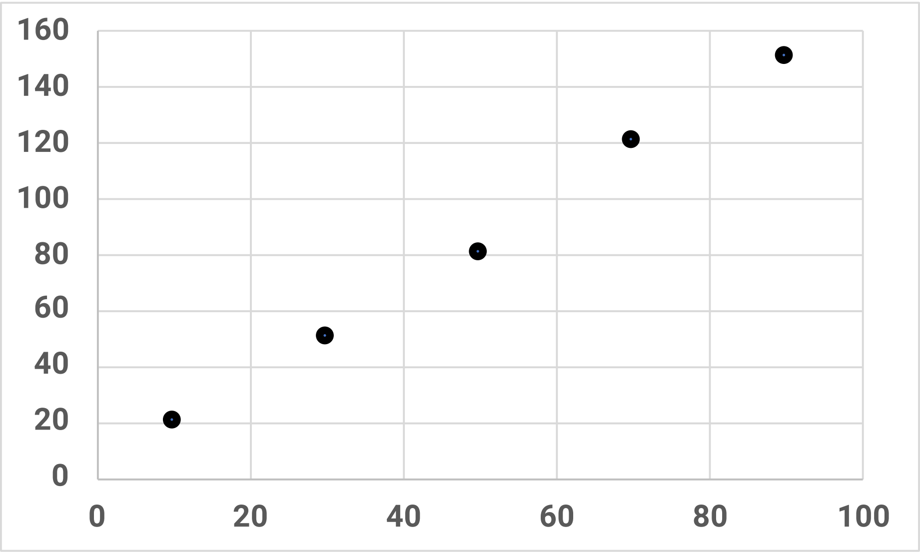
$y = 5 \times 10^6 \sin x / (x^2 + 2)$

$y = ax + b$

$a = \dfrac{y_2 - y_1}{x_2 - x_1}$ $\quad b = \begin{cases} y_1 - ax_1 \\ y_2 - ax_2 \end{cases}$

Data representation & analysis

10	20
30	50
50	80
70	120
90	150



$y = mx + c$

$m = \dfrac{y_2 - y_1}{x_2 - x_1}$

$= \dfrac{150 - 20}{90 - 10}$

$= 1.625$

$c = y_1 - mx_1 = 20 - 1.625 \times 10 = 3.75$

$y = 1.625x + 3.75$

$y_2 = 1.625 \times 90 + 3.75 = 150$

Nonlinear data

$$y = mx^2 + c$$

$$y^2 = \frac{m}{x} + c$$

$$\frac{1}{y} = m\left(x + 3\right) + c$$

$$\sin y = m\left(x^2 - 4\right)$$

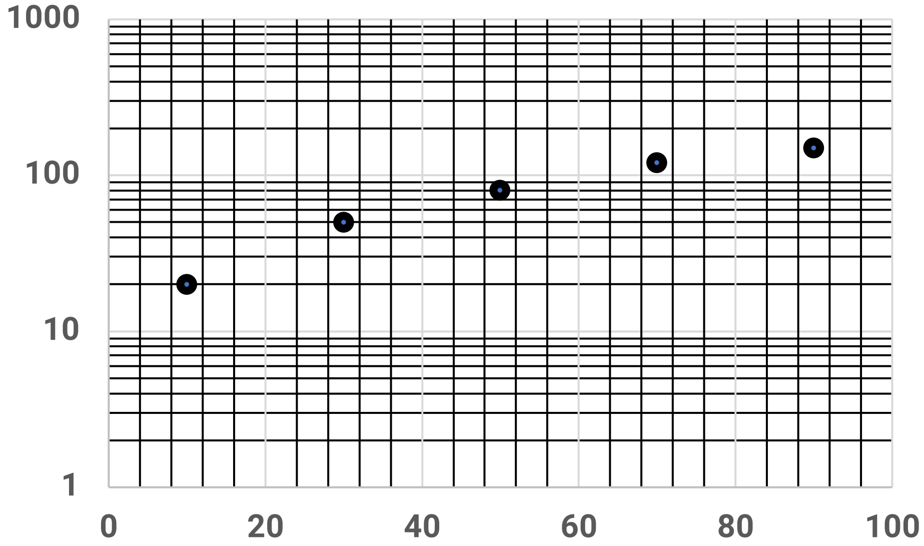
$$y = \frac{1}{m_1 x - c}$$

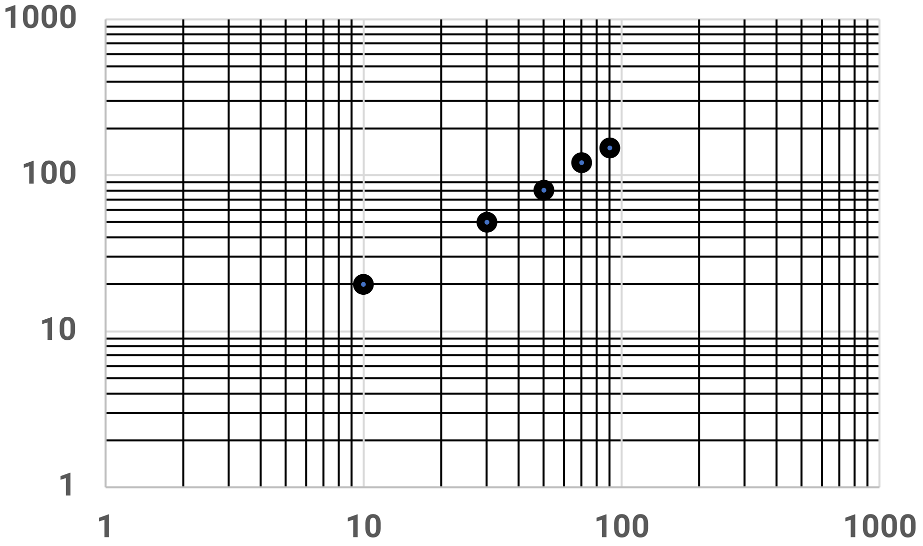
$$\Rightarrow \frac{1}{y} = m_1 x - c$$

$$y = 1 + x\left(mx^2 + c\right)^{1/2}$$

$$\Rightarrow \frac{\left(y - 1\right)^2}{x^2} = mx^2 + c$$

Nonlinear data





Validating results

- back-substitution
- order-of-magnitude estimation
- test of reasonableness

Processes & Process Variables

- Process: operation to achieve desired product
  - input - feed, output – product, process streams
  - design – flowchart
  - operation – daily activities
  - analysis – intensification
  - troubleshooting – problem identification
  - debottlenecking – scale up
  - turndown – scale down
- Understanding composition, process condition
  - process variables

Process Variables

- Density / specific volume
- Specific gravity (SG)
  - reference fluid – water at 4.0 ^{0}C (1000 kg/m^3)
- Mass & volume flow rate
- Chemical composition
  - moles & molecular weight
  - mass and mole fractions, & average molecular weight
  - concentration
  - parts per million (ppm) and parts per billion (ppb)

Chemical Composition

- Gram-mole (g-mole or mol) - amount of species whose mass in grams is numerically equal to its molecular weight
  - kg/kmol, g/mol, and lb_m/lb-mole
- Same conversion factors for molar units that are used to convert masses from one unit to another

$$100\ g\ CO_2 \times \frac{1\ mol\ CO_2}{44\ g\ CO_2} = 2.273\ mol\ CO_2$$

$$2.273\ mol \times \frac{1\ lb\text{-}mol}{453.6\ mol} = 5.011 \times 10^{-3}\ lb.mol$$

Chemical Composition

$$2.273 \text{ mol } CO_2 \times \frac{1 \text{ mol } C}{1 \text{ mol } CO_2} = 2.273 \text{ mol } C$$

$$2.273 \text{ mol } CO_2 \times \frac{1 \text{ mol } O_2}{1 \text{ mol } CO_2} = 2.273 \text{ mol } O_2$$

$$2.273 \text{ mol } CO_2 \times \frac{2 \text{ mol } O}{1 \text{ mol } CO_2} = 4.546 \text{ mol } O$$

$$4.546 \text{ mol } O \times \frac{16.0 \text{ g } O}{1 \text{ mol } O} = 72.7 \text{ g } O$$

$$2.273 \text{ mol } O_2 \times \frac{32.0 \text{ g } O_2}{1 \text{ mol } O_2} = 72.7 \text{ g } O_2$$

$$100.0 \text{ g } CO_2 \times \frac{32.0 \text{ g } O_2}{44.0 \text{ g } CO_2} = 72.7 \text{ g } O_2$$

Chemical Composition

- molecular weight can be used to relate the mass flow rate to the corresponding molar flow rate

$$\frac{100 \text{ kg } CO_2}{h} \times \frac{1 \text{ kmol } CO_2}{44.0 \text{ kg } CO_2} = 2.27 \frac{\text{kmol } CO_2}{h}$$

- **dalton (Da)** ⇒ molecular weight and the size of molecules for biochemical species
- The mass of a carbon-12 atom = 12 daltons
- The mass of a water molecule = 18 daltons

Chemical Composition

- Mass fraction (x)
  - mass of a species / total mass of mixture
- Mole fraction (y)
  - moles of a species / total moles of mixture

$$\boxed{\begin{array}{l} x_A = 0.15 \\ y_B = 0.20 \end{array}}$$

for 175 kg solution

mass of A = 175 × 0.15 kg = 26 kg A

for the solution flow rate of 1000 mol/min

molar flow rate of B = 200 mol B/min

Mass & Molar Composition

Component	Mass Fraction	Mass (g)	Molecular Weight	Moles	Mole Fraction
i	x_i (g_i / g)	$m_i = x_i\, m_{\mathrm{total}}$	M_i (g/mol)	$n_i = m_i/M_i$	$y_i = n_i = n_{\mathrm{total}}$
O_2	0.16	16	32	0.50	0.15
CO	0.04	4	28	0.14	0.04
CO_2	0.17	17	44	0.39	0.12
N_2	0.63	63	28	2.25	0.69
Total	**1.00**	**100**		**3.28**	**1.00**

Texts

- **BASIC PRINCIPLES AND CALCULATIONS IN CHEMICAL ENGINEERING**
  - David M. Himmelblau and James B. Riggs
  - Prentice Hall

- **ELEMENTARY PRINCIPLES OF CHEMICAL PROCESSES**
  - Richard M. Felder and Ronald W. Rousseau
  - John Wiley & Sons, Inc.

CHEMICAL PROCESS CALCULATIONS

Lecture #3: August 10, 2023

Chemical Composition

- Mass fraction (x)
  - mass of a species / total mass of mixture
- Mole fraction (y)
  - moles of a species / total moles of mixture

$\boxed{\begin{array}{l} x_A = 0.15 \\ y_B = 0.20 \end{array}}$

for 175 kg solution

mass of A = 175 × 0.15 kg = 26 kg A

for the solution flow rate of 1000 mol/min

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Mass & Molar Composition

Component	Mass Fraction	Mass (g)	Molecular Weight	Moles	Mole Fraction
i	x_i (g_i / g)	$m_i = x_i\, m_{\text{total}}$	M_i (g/mol)	$n_i = m_i/M_i$	$y_i = n_i = n_{\text{total}}$
O_2	0.16	16	32	0.50	0.15
CO	0.04	4	28	0.14	0.04
CO_2	0.17	17	44	0.39	0.12
N_2	0.63	63	28	2.25	0.69
Total	**1.00**	**100**		**3.28**	**1.00**

Average Molecular Weight

- Ratio of mixture mass and number of moles of all species

$$\overline{M} = y_1 M_1 + y_2 M_2 + \ldots . = \sum y_i M_i$$

$$\frac{1}{\overline{M}} = \frac{x_1}{M_1} + \frac{x_2}{M_2} + \ldots . = \sum \frac{x_i}{Mi}$$

Molar composition: 79% N_2 & 21% O_2
Mass composition: 76.7% N_2 & 23.3% O_2

$$\overline{M} = y_{N_2} M_{N_2} + y_{O_2} M_{O_2}$$

$$= 0 \cdot 79 \times 28 + 0 \cdot 21 \times 32$$

$$= 29 \frac{kg}{kmol}$$

Average Molecular Weight

- Ratio of mixture mass and number of moles of all species

$$\overline{M} = y_1M_1 + y_2M_2 + \ldots. = \sum y_iM_i$$

$$\frac{1}{\overline{M}} = \frac{x_1}{M_1} + \frac{x_2}{M_2} + \ldots. = \sum \frac{x_i}{Mi}$$

Molar composition: 79% N_2 & 21% O_2
Mass Composition: 76.7% N_2 & 23.3% O_2

$$\frac{1}{\overline{M}} = \left(\frac{0\cdot 767}{28} + \frac{0\cdot 233}{32}\right)\frac{mol}{g}$$

$$= 0.035\frac{mol}{g}$$

$$\Rightarrow \overline{M} = 29\frac{g}{mol}$$

Concentration

- Mass and Molar concentration
  - mass and number of moles per unit volume of the mixture
  - **molarity** - molar concentration of the solute in gram-moles solute/liter solution
  - parts per million (ppm) and parts per billion (ppb)
    - parts (grams, moles) of the species per million or billion parts
    - used for trace species
    - ppm = $y \times 10^6$
    - ppb = $y \times 10^9$

Pressure

- Absolute pressure: zero for vacuum
- Gauge pressure: pressure relative to atmospheric pressure
- Absolute pressure = Gauge pressure + Atmospheric pressure

Process Classification

- Batch process
- Continuous process
- Semi-batch process

- Steady state
- Transient or unsteady-state

General Balance Equation

Input + generation = output + consumption + accumulation

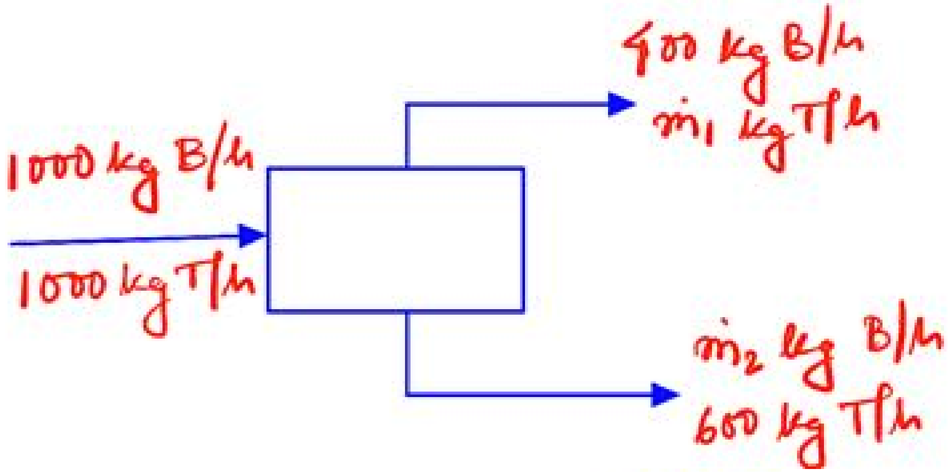
General Balance Equation

- **Differential balances (normally applied to continuous process)**
  - describe at an instant in time
  - each term represents the rate of input, rate of generation, etc.
- **Integral balances (normally applied to batch process)**
  - describe between two instants of time
  - each term represents the amount of the balanced quantity
- When balanced parameter = total mass
  - generation = 0 and consumption = 0 (except in nuclear reactions)
- When balanced parameter = nonreactive species
  - generation = 0 and consumption = 0
- When the system is at steady state
  - accumulation = 0 (always!)

Continuous Steady-State Processes

- input + generation = output + consumption
- for total mass or non-reactive species
  - input = output
- Two thousand kilograms per hour of a mixture of benzene (B) and toluene (T) containing 50% benzene by mass is separated into two fractions. The mass flow rate of benzene in one stream is 400 kg B/h and that of toluene in the other stream is 600 kg T/h. The operation is at steady state. Write balances on benzene and toluene to calculate the unknown component flow rates in the output streams.

Continuous Steady-State Processes



Input = Output

Benzene balance

$$1000 \text{ kg B/h} = 400 \text{ kg B/h} + \dot{m}_2 \text{ kg B/h}$$

$$\Rightarrow \dot{m}_2 = 600 \text{ kg B/h}$$

Toluene Balance:

$$1000 \text{ kg T/h} = \dot{m}_1 \text{ kg T/h} + 600 \text{ kg T/h}$$

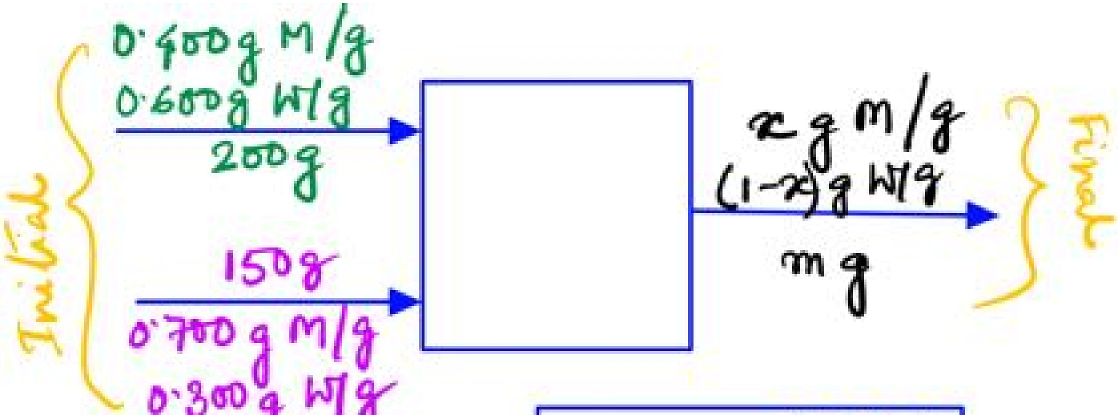
$$\Rightarrow \dot{m}_1 = 400 \text{ kg T/h}$$

Batch Processes

- accumulation = final output - initial input

  = generation - consumption
- initial input + generation = final output + consumption

There are two methanol–water mixtures in separate flasks. The first mixture contains 40.0 wt% methanol, and the second contains 70.0 wt% methanol. If 200 g of the first mixture is combined with 150 g of the second, what are the mass and composition of the product?



$$\boxed{\text{Input} = \text{Output}}$$

Total mass balance:

$$200\,g + 150\,g = m$$

$$\Rightarrow m = 350\,g$$

Methanol balance:

$$200 \times 0{\cdot}400 + 150 \times 0{\cdot}700 = m \times x = 350x$$

$$\Rightarrow x = 0{\cdot}529\ g\ M/g$$

$$\Rightarrow 1 - x = 0{\cdot}471\ g\ W/g$$

Texts

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CHEMICAL PROCESS CALCULATIONS

Lecture #4: August 14, 2023

General Balance Equation

Input + generation = output + consumption + accumulation

General Balance Equation

- **Differential balances (normally applied to continuous process)**
  - describe at an instant in time
  - each term represents the rate of input, rate of generation, etc.
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Continuous Steady-State Processes

- input + generation = output + consumption
- for total mass or non-reactive species
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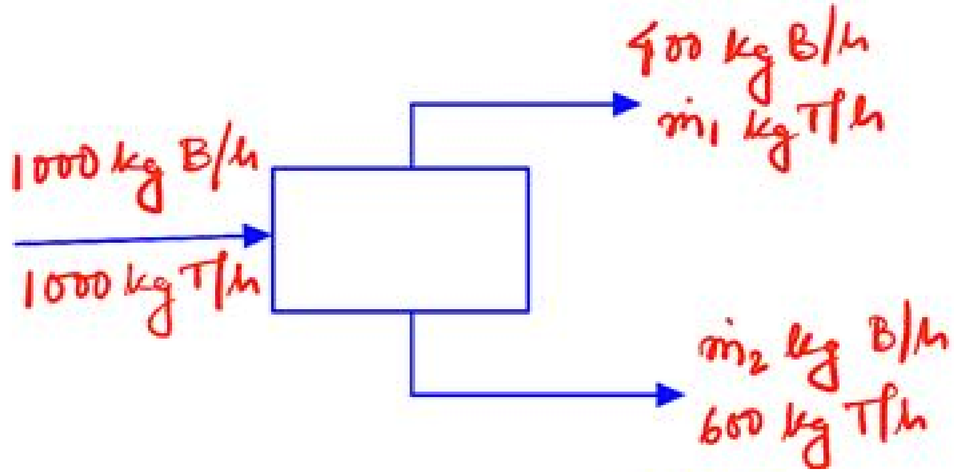
- Two thousand kilograms per hour of a mixture of benzene (B) and toluene (T) containing 50% benzene by mass is separated into two fractions. The mass flow rate of benzene in one stream is 400 kg B/h and that of toluene in the other stream is 600 kg T/h. The operation is at steady state. Write balances on benzene and toluene to calculate the unknown component flow rates in the output streams.

Continuous Steady-State Processes



Input = Output

Benzene balance

$$1000 \text{ kg B/h} = 400 \text{ kg B/h} + \dot{m}_2 \text{ kg B/h}$$

$$\Rightarrow \dot{m}_2 = 600 \text{ kg B/h}$$

Toluene Balance:

$$1000 \text{ kg T/h} = \dot{m}_1 \text{ kg T/h} + 600 \text{ kg T/h}$$

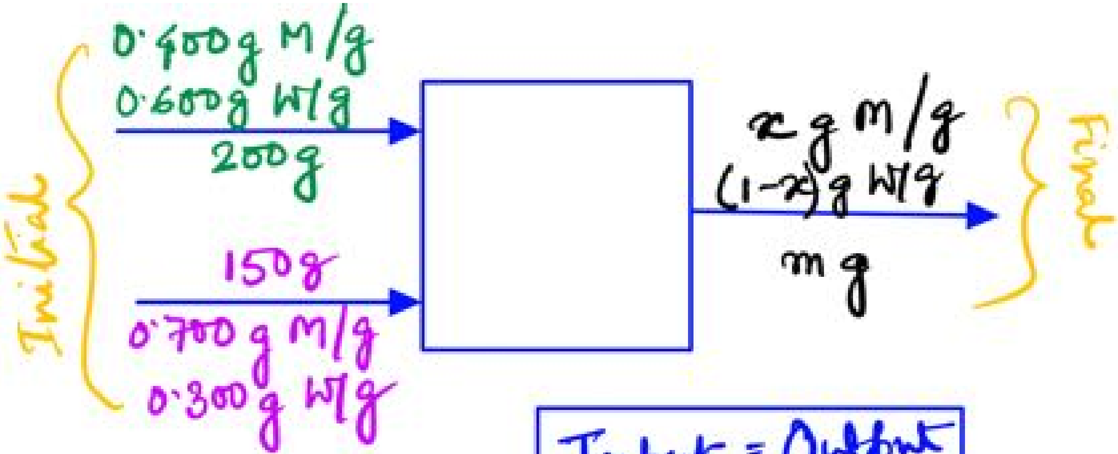
$$\Rightarrow \dot{m}_1 = 400 \text{ kg T/h}$$

Batch Processes

- accumulation = final output - initial input

  = generation - consumption
- initial input + generation = final output + consumption

There are two methanol–water mixtures in separate flasks. The first mixture contains 40.0 wt% methanol, and the second contains 70.0 wt% methanol. If 200 g of the first mixture is combined with 150 g of the second, what are the mass and composition of the product?



$$\boxed{\text{Input} = \text{Output}}$$

Total mass balance:

$$200\,g + 150\,g = m$$

$$\Rightarrow m = 350\,g$$

Methanol balance:

$$200 \times 0{\cdot}400 + 150 \times 0{\cdot}700 = m \times x = 350x$$

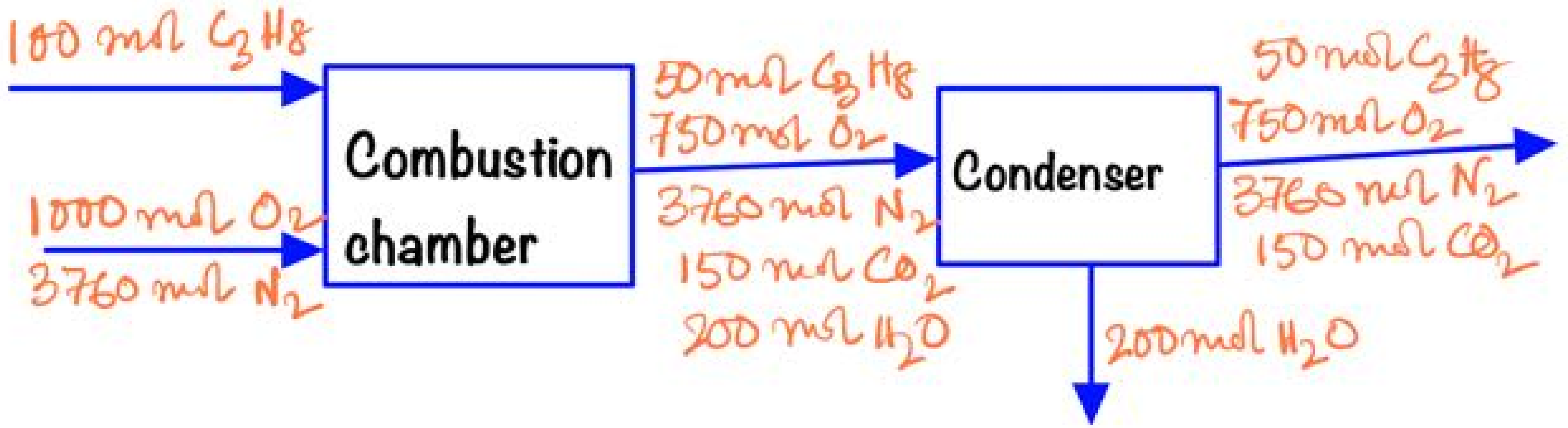
$$\left.\begin{aligned} &\Rightarrow x = 0{\cdot}529\ g\ M/g \\ &\Rightarrow 1 - x = 0{\cdot}471\ g\ W/g \end{aligned}\right\}$$

Flowchart

- Boxes/symbols for process units
  - reactors, mixers, separation units, etc.
- Lines + arrows for inlets and outlets
- A gas mixture containing N_2 & O_2 is combusted with propane (C_3H_8) in a batch combustion chamber. Some of the O_2 and C_3H_8 react to form CO_2 and H_2O, and then the product is cooled for condensing the water.

Flowchart

- A gas mixture containing N_2 & O_2 is combusted with propane (C_3H_8) in a batch combustion chamber. Some of the O_2 and C_3H_8 react to form CO_2 and H_2O, and then the product is cooled for condensing the water.



Flowchart

400 mol/h

$\longrightarrow$

0·21 mol O_2/mol

0·79 mol N_2/mol

$T = 350°C$, $P = 1·5$ atm

60 mol N_2/min

$\longrightarrow$

40 mol O_2/min

$\Leftrightarrow$

100 mol/min

$\longrightarrow$

0·6 mol N_2/mol

0·4 mol O_2/mol

Flowchart

$\dot{n}$ (mol/h)

0.21 mol O_2/mol
0.79 mol N_2/mol
T = 350°C, P = 1.5 atm

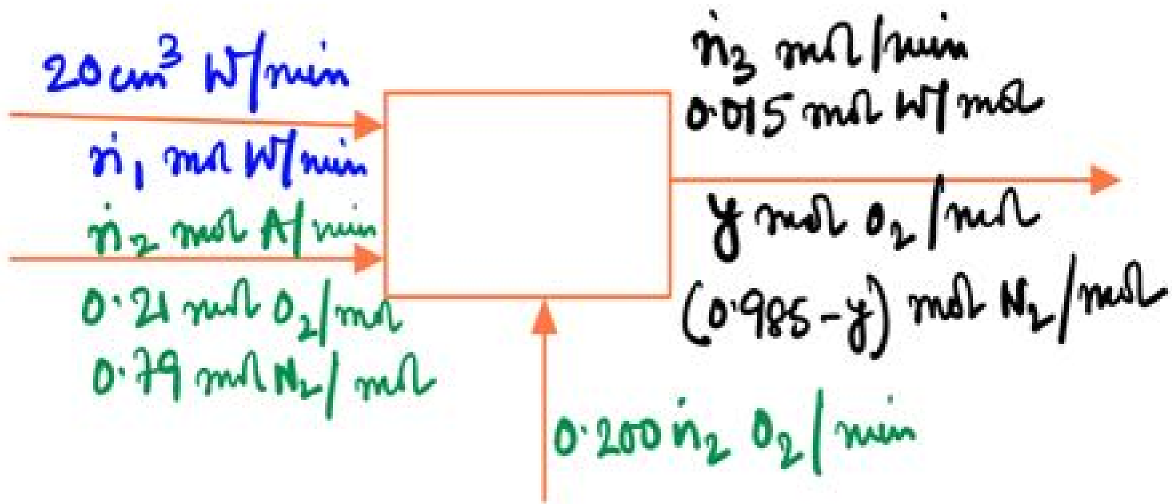
400 mol/h

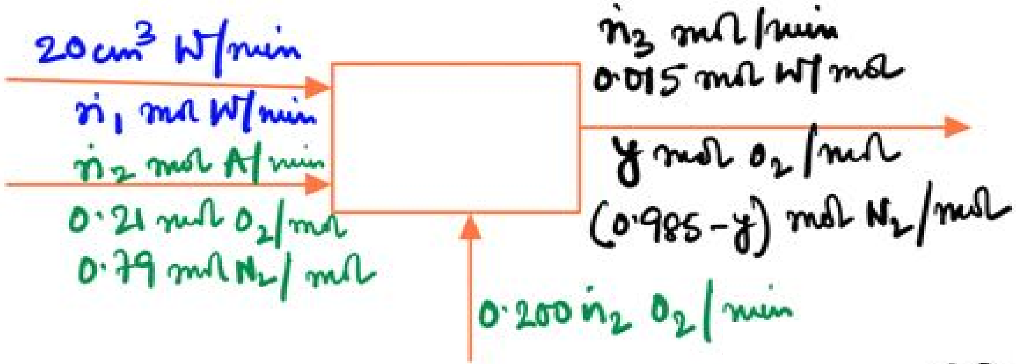
y mol O_2/mol
(1 - y) mol N_2/mol
T = 350°C, P = 1.5 atm

An experiment on the growth rate of certain organisms requires an environment of humid air enriched in oxygen. Three input streams are fed into an evaporation chamber to produce an output stream with the desired composition.

A: Liquid water, fed at a rate of 20.0 cm^3/min
B: Air (21 mole% O_2, the balance N_2)
C: Pure oxygen, with a molar flow rate one-fifth of the molar flow rate of stream B

The output gas is analyzed and is found to contain 1.5 mole% water. Draw and label a flowchart of the process, and calculate all unknown stream variables.





unit consistency

$$\dot{n}_1 = \frac{20.0\ cm^3\ H_2O}{min} \times \frac{1.00\ g\ H_2O}{cm^3} \times \frac{1\ mol}{18\ g}$$

$$\Rightarrow \dot{n}_1 = 1.11\ \frac{mol\ H_2O}{min}$$

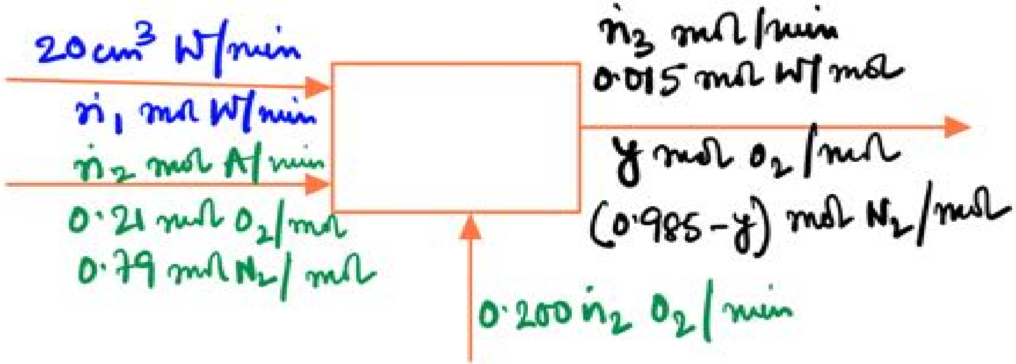
Nonreactive Steady State process

Input = Output

H_2O (W) balance:

$$\dot{n}_1 = \dot{n}_3 \times 0.015$$

$$\Rightarrow \dot{n}_3 = 1.11/0.015 = 74\ \frac{mol}{min}$$



Total mole balance:

$$\dot{n}_1 + \dot{n}_2 + 0.200\,\dot{n}_2 = \dot{n}_3$$

$$\Rightarrow \quad \dot{n}_2 = (74 - 1.11)/1.200 \text{ mol/min}$$

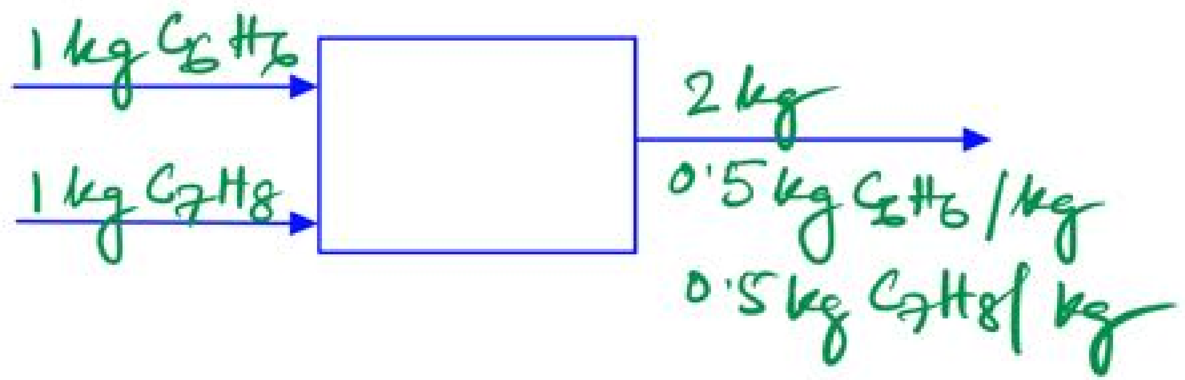
$$= 61 \frac{\text{mol}}{\text{min}}$$

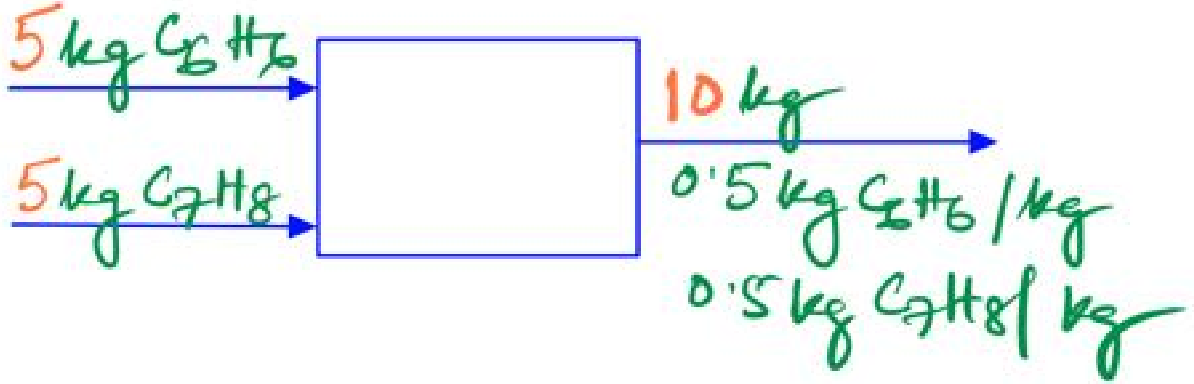
N_2 balance:

$$\dot{n}_2 \times 0.79 = \dot{n}_3 \times (0.985 - y)$$

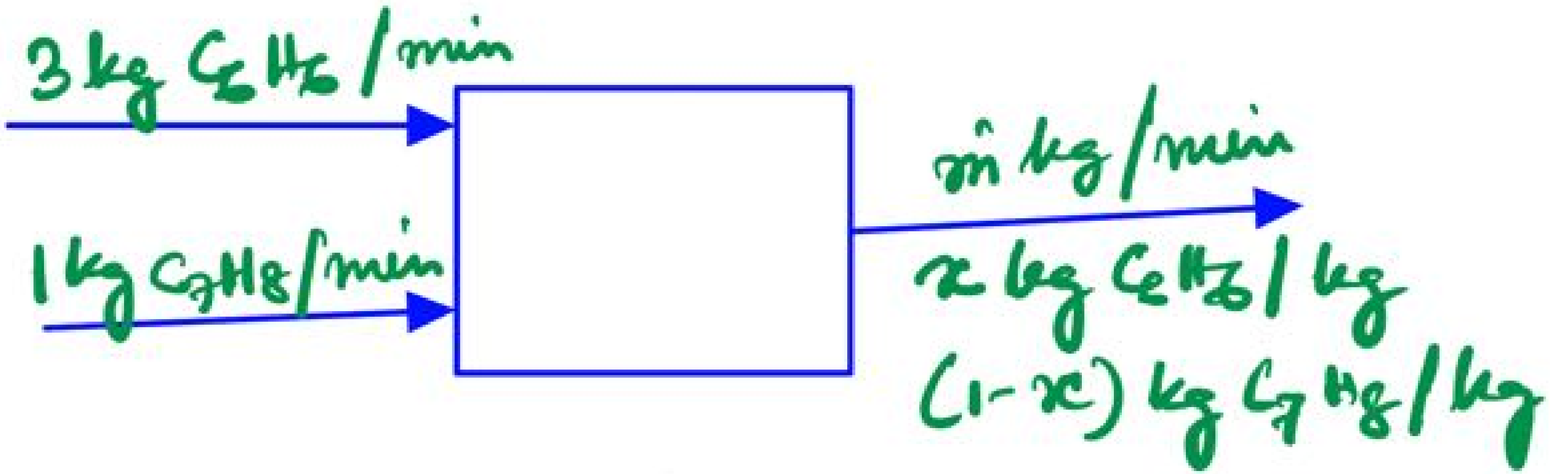
$$\Rightarrow \quad y = 0.33 \text{ mol } O_2/\text{mol}$$

Flowchart scaling





Writing balance equations



Total Mass Balance

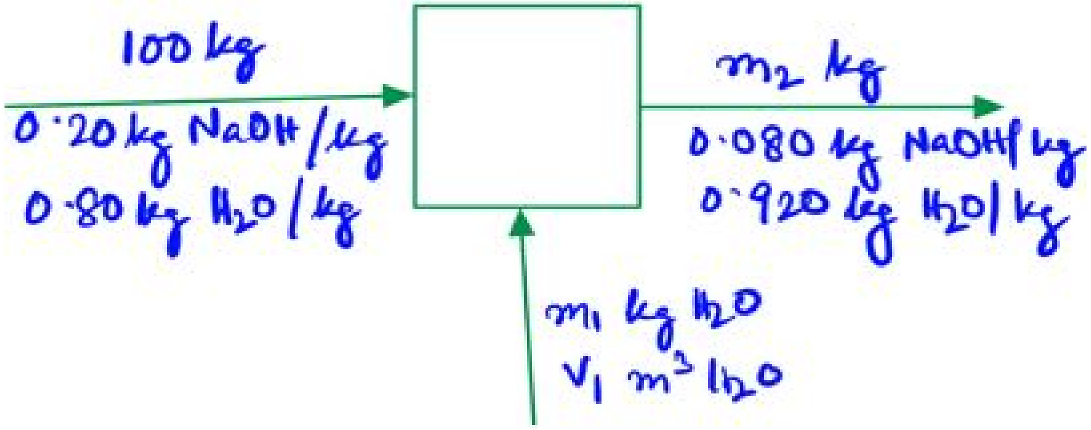
$$3 + 1 = \dot{m} \Rightarrow \dot{m} = 4 \text{ kg/min}$$

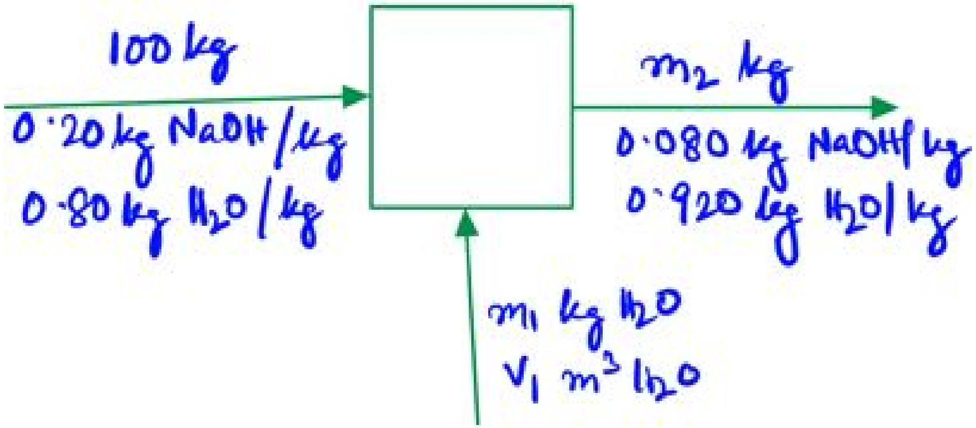
Benzene Balance

$$3 = \dot{m} \times x \Rightarrow x = 0.75 \text{ kg } C_6H_6/\text{kg}$$

Writing balance equations

- For a nonreactive system:
  - maximum number of independent equations = the number of chemical species in the input and output streams
- Priority for the balance which has the fewest unknown variables





Basis of calculation
Desired variables
unknowns
equations
solution procedure

Total mass balance

$$100 + m_1 = m_2 \Rightarrow m_1 = 150 \text{ kg } H_2O$$

$$\rho_{H_2O} = 1000 \text{ kg}/m^3$$

$$\Rightarrow V_1 = 150/1000 \ m^3 = 0.15 \ m^3$$

NaOH Balance

Input = Output

$$0.20 \times 100 = 0.080 \times m_2$$

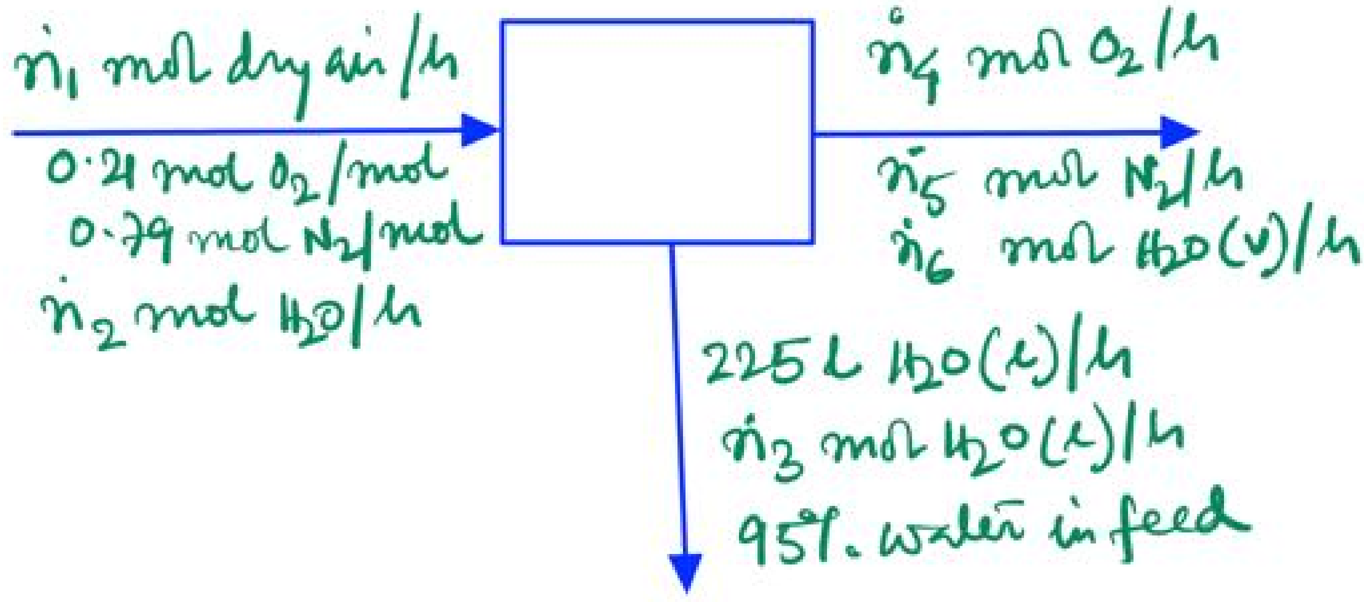
$$\Rightarrow m_2 = 250 \text{ kg NaOH}$$

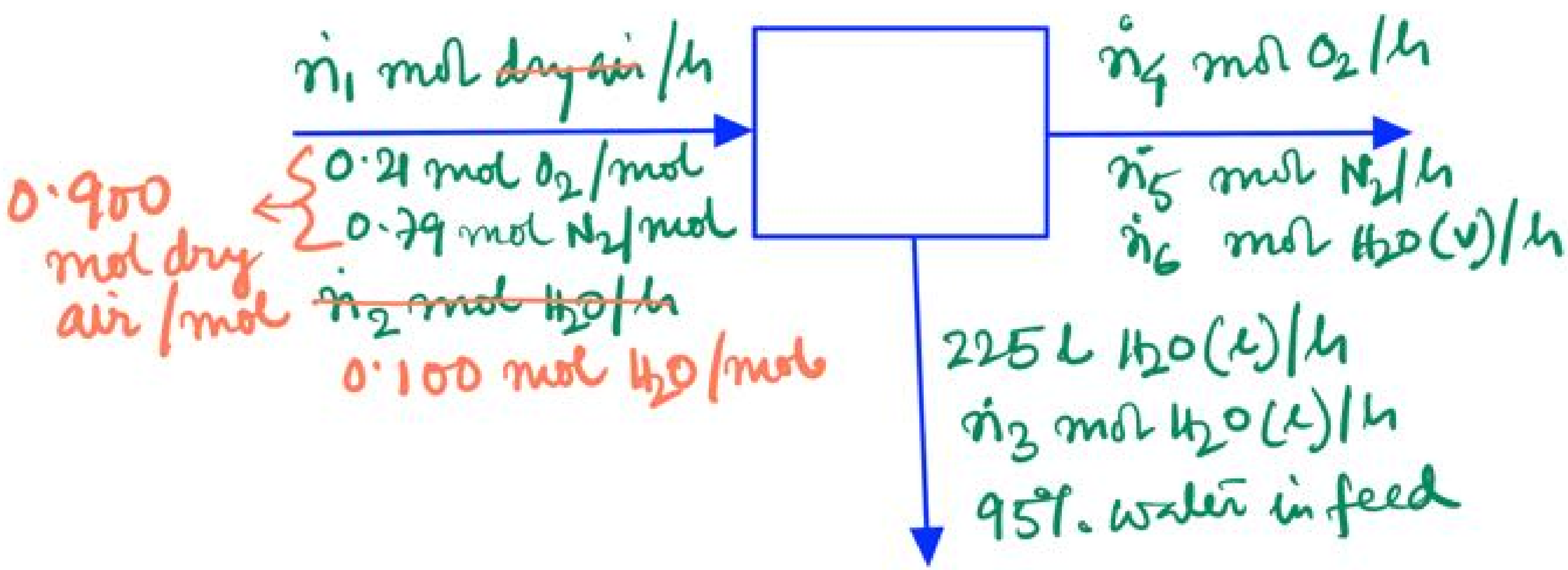
Degree-of-Freedom Analysis

- Draw and completely label the flowchart
- Count the unknown variables
- Count the independent equations relating them
- Subtract the second number from the first

Degree-of-Freedom Analysis

A stream of humid air enters a condenser in which 95% of the water vapor in the air is condensed. The flow rate of the condensate (the liquid leaving the condenser) is measured and found to be 225 L/h. Dry air may be taken to contain 21 mole% oxygen, with the balance nitrogen. Calculate the flow rate of the gas stream leaving the condenser and the mole fractions of oxygen, nitrogen, and water in this stream.




$\dot{n}_1$ mol ~~dry air~~/h
0.21 mol O_2/mol
0.79 mol N_2/mol
0.900 mol dry air/mol
~~$\dot{n}_2$ mol H_2O/h~~
0.100 mol H_2O/mol
$\dot{n}_4$ mol O_2/h
$\dot{n}_5$ mol N_2/h
$\dot{n}_6$ mol H_2O(v)/h
225 L H_2O(l)/h
$\dot{n}_3$ mol H_2O(l)/h
95% water in feed

Single-Unit Process Calculations

1. Choose a basis
2. **Draw and label the flowchart**
3. Write expressions for the quantities asked in the problem statement
4. Convert mixed units to one basis
5. **Perform degree-of-freedom analysis**
6. Write system equations and outline a solution procedure
7. Calculate the unknowns
8. Calculate ***additional quantities*** requested in the problem statement

Texts

- **BASIC PRINCIPLES AND CALCULATIONS IN CHEMICAL ENGINEERING**
  - David M. Himmelblau and James B. Riggs
  - Prentice Hall

- **ELEMENTARY PRINCIPLES OF CHEMICAL PROCESSES**
  - Richard M. Felder and Ronald W. Rousseau
  - John Wiley & Sons, Inc.