# CE407 SEPARATIONS

Lecture 01

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# Separations

- In the chemical industry we often have homogenous mixtures of chemicals that cannot be separated by mechanical means
  - Mechanical means are things like filters
- This course will look at methods that exploit thermodynamic equilibrium to separate materials
- Motivation
  1. Purify a product by removing impurities
  2. Extract the product from a mixture
  3. Remove potentially harmful agents before releasing a stream to the atmosphere

# Terminology

- Solute
  - This is the component you are trying to transfer, either because
    - It is the product you want in a purified form or
    - It is a contaminant you want to eliminate
- x typically refers to a mole fraction in a liquid phase
- y typically refers to a mole fraction in a vapor phase (gas phase)
- Do NOT confuse the term vapor as referring to a mist or steam – in this course it means a gaseous phase
- Mole Fractions are typically used when we are working through the physics
- Mass Fractions or ratios are sometimes used when we are using experimental data
  - Leaching and Liquid-Liquid Extraction

# Mole Fractions

- Defined as:

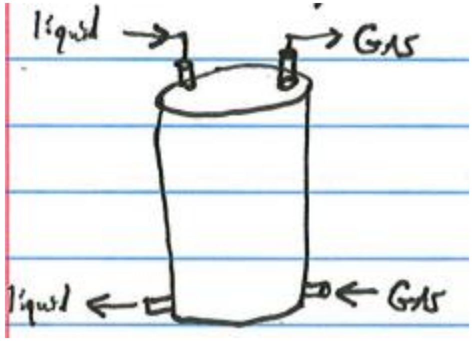
$$x_i = \frac{\#\ of\ moles\ of\ component\ i\ in\ liquid\ phase}{total\ \#\ of\ moles\ in\ liquid\ phase}$$

$$x_i = \frac{\#\ of\ moles\ of\ component\ i\ in\ liquid\ phase}{\#\ of\ moles\ of\ component\ i\ in\ liquid\ phase + \#\ of\ moles\ of\ carrier\ in\ liquid\ phase}$$

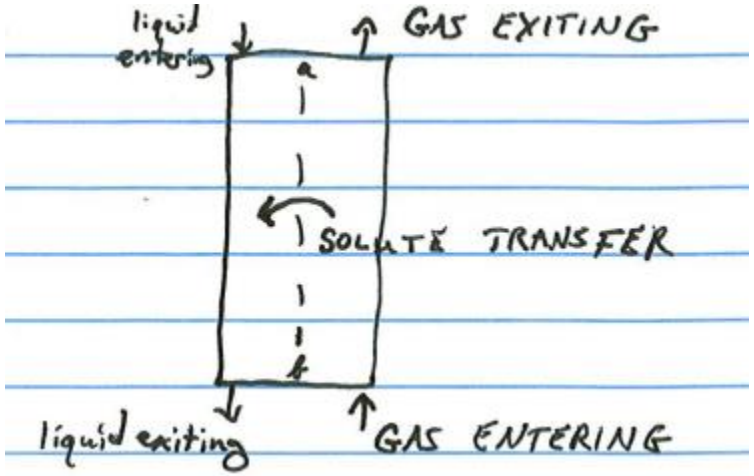
- Similar definition for $y_i$
- i refers to the component
  - Component 1 versus component 2, etc

# Gas Absorption

- Typically occurs in a cylindrical tower




- We will symbolically depict this as this side view:
- a is the top of the tower and b is the bottom
- The gas goes up the tower and the liquid flows down
  - That is actually what happens – due to gravity!
- The flows are not actually one phase going down the left hand side and the other phase going up the right hand side
- Flows go over or through trays or packing to maximize contact

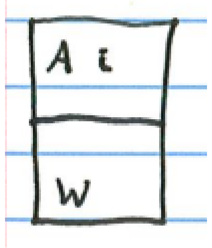


# Gas Absorption – What’s Happening?

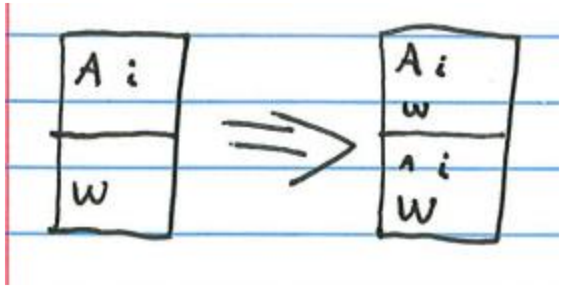
- We have a mixture of components that cannot be mechanically separated
  - Benzene vapor in air
- We introduce another material which in a different phase (liquid versus gas)
- If the solute is in a lower energy state when it is in the newly introduced phase, mass transfer will occur and the solute will transfer into the new material
- Because the new material is a different phase from the original material it will naturally separate from the original mixture
- This results in the removal of the solute from the original mixture

# Single Stage Absorption Analysis

- **Initial state**
  - i is solute
  - A is air
  - W is water
  - Water is introduced to gas mixture of solute and air




- **Complete Case**
  - Some water evaporates into air
  - Some air dissolves into the water
  - Solute is distributed between the two phases
  - Relative size of the symbols indicates general order of magnitude
  - Experience shows that the air dissolving into the water is not a large enough mole fraction to affect the calculations
  - Note that it is likely that the water already had air dissolved in it to begin with



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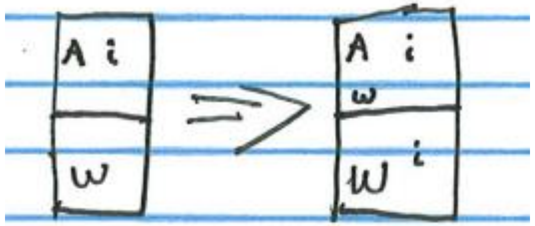
# Single Stage Absorption Analysis, continued

- **“Rigorous” Case**
  - Ignores dissolution of air into the water
  - Does consider the evaporation of water into air
  - Of course, the distribution of the solute is included
  - Air, water, and solute will be in vapor phase
  - Water and solute in liquid phase




- **“Usual Assumptions” Case**
  - Ignores evaporation of water into air
  - Ignores dissolution of air into water
  - Of course, the distribution of the solute is included
  - Air and solute in the vapor phase
  - Water and solute in the liquid phase

# Single Stage Absorption Analysis, continued

- Which model is "best"?
- See Notes titled **"Single Stage Absorption"** for mathematical analysis of "Rigorous" versus "Usual Assumptions" cases
- The analysis shows that the simpler "Usual Assumptions" case does an excellent job of predicting the mole fraction of solute in both phases
- The simpler "Usual Assumptions" case does an extraordinarily bad job of predicting the mole fraction of water in the vapor phase
  - We are seldom concerned with knowing the water content of the vapor leaving the tower…

# Equilibrium Relationships

- Used to calculate mole fractions of distributed components (i.e. components that are being transferred from one phase to another)

- **Raoult's Law**

$$y_i P = x_i P_i^{sat}(T)$$

- $P_i^{sat}(T)$ is the vapor pressure of the solute. It is **STRONGLY** dependent on temperature
- Note that interactions between the solute and solvents is ignored

# Equilibrium Relationships, continued

- **Generalized Equilibrium Relationship**

$$y_i P = x_i \gamma_i P_i^{sat}(T)$$

- $\gamma_i$ is the Activity Coefficient, which accounts for interactions between the solvent and the solute
  - It is STRONGLY dependent on the composition of the mixture and the temperature
- Gas phase is still considered ideal (molecules are separated by great distances)

# Equilibrium Relationships, continued

- **Henry's Law**
- For cases where $x_i$ << 1 (say 0.01 or lower)

$$y_i P = x_i \gamma_i^{\infty} P_i^{sat}(T)$$

$\gamma_i^{\infty}$ is Infinite Dilution activity coefficient and is considered to be relatively constant in the very dilute range for a given temperature

- $k_i(T) = \gamma_i^{\infty} P_i^{sat}(T)$
- $k_i(T)$ is Henry's Law coefficient and is temperature dependent
- Henry's Law acknowledges that the ideality assumed in Raoult's Law is not accurate, but assumes that in the case of a dilute solution the dependence on composition can be ignored