ChE211.1: Introduction to Chemical Engineering

Fundamentals of chemical reaction calculations

Ayoade Kuye

Learning Objectives

- Understand the main goals of chemical process engineering and the metrics used to quantify progress towards these goals:
  - Volumetric Productivity; Yield vs. Atom Economy; Purity
- Recognize four types of chemical processes (batch, continuous, semi-batch, and semi-continuous) and their relative pros and cons.

Introduction

- Chemical reactions transform substances into new substances with different physical and chemical properties.
  - occur when the bonds between atoms in molecules are broken or formed, resulting in the rearrangement of atoms and the creation of new chemical bonds.
  - are described by chemical equations (the reactants and products of the reaction as well as the stoichiometry of the reaction). Balancing chemical equations is a key concept in chemical reactions, as it ensures that the number of atoms of each element is conserved in the reaction.

Introduction

- Examples of chemical reactions include
  - ✓Combustion reactions, in which a fuel reacts with oxygen to produce heat and light.
  - ✓Acid-base reactions, in which an acid and a base react to produce salt and water.
  - ✓Redox reactions, in which electrons are transferred between reactants, result in oxidation state changes.
  - ✓Precipitation reactions, in which two aqueous solutions react to form an insoluble solid.
  - ✓Complexation reactions, in which a metal ion is bound to a ligand to form a complex.

Fundamentals of chemical reaction calculations

- Stoichiometry is the quantitative study of chemical reactions.
  - The calculation of quantities of reactants and products involved in a chemical reaction based on principles of conservation of mass and the laws of chemical combination.
- Equivalents: the amount of one substance that reacts with one mole of another substance.
  - This will often (but not always) be a 1:1 mole ratio.
- Mole Percent: typically used when considering mixtures of different chemicals.
  - $\text{Mol \%} = 100 \text{ x } \frac{\text{Moles of substance of interest}}{\text{Total moles}}$
- Percent Excess: typically used when considering chemical reactions in which one reactant is present in limiting quantities and the other(s) are in excess.
  - $\mathbf{\% \text{ Excess} = 100 \text{ x } \frac{\text{Actual moles of reactant} - \text{stoichiometrically required moles of reactant}}{\text{stoichiometrically required moles of reactant}}}$

Goal of a Chemical Process Engineer

- Find the optimal balance between maximizing **productivity** and **product quality**, while minimizing **waste**
- **How to measure productivity?**
  - Volumetric Productivity = amount of product generated by the bottlenecking unit operation per unit volume per unit time (with units typically "g/L-h" or "mol/L-h"). This is sometimes referred to as "space-time-yield".
  - Time is important because of capital costs of equipment. In extreme case, if raw material is cheap and product is expensive, cost of goods (CoGs) is primarily dictated by duration of use of a modularly designed, multipurpose chemical plant.

Goal of a Chemical Process Engineer

- Find the optimal balance between maximizing **productivity** and **product quality**, while minimizing **waste**
- **How to measure waste?**
  - Yield:
    - ✓Traditionally, "yield" has been used as the primary metric for measuring waste
      - $Yield = 100\ x\ \frac{Actual\ Yield}{Theoretical\ Yield}$
    - ✓"Theoretical yield" is the amount (mass or moles) of product that would be formed if all of the limiting reactant was converted to product.

Goal of a Chemical Process Engineer

- Find the optimal balance between maximizing **productivity** and **product quality**, while minimizing **waste**
- **How to measure waste?**
  - Atom Economy:
    - ✓A better way to measure the conversion e?iciency of a chemical process is according to the principle of "Atom Economy".

$$Atomic\ Economy = 100\ x\ \frac{Molecular\ weight\ of\ desired\ product}{Formular\ weights\ of\ all\ the\ atoms\ in\ reactants} = \frac{MW_{Product}}{\sum FW_{all\ reactants}}$$

Goal of a Chemical Process Engineer

- Atom Economy Example:

Which of the following reactions is most likely to be the foundation of a state-of-the-art chemical process for making phenol? Why?

a) $C_6H_6 + H_2SO_4 + 2NaOH \rightarrow C_6H_5OH + Na_2SO_3 + 2H_2O$

b) $C_6H_6 + N_2O \rightarrow C_6H_5OH + N_2$

c) $C_6H_5CH_3 + 2O_2 \rightarrow C_6H_5OH + CO_2 + H_2O$

$$A.E = \frac{MW_{prod}}{\sum FW_{all\ atoms,react}} \times 100\%$$

(a) $MW_{prod} = 6(12) + 6(1) + 16 = 94\ g/mol$

$\sum FW = 6(12) + 10(1) + 32 + 6(16) + 2(23) = 256\ g/mol$

$\frac{94}{256} \times 100\% = 37\%$

(b) $\sum FW = 6(12) + 6(1) + 2(14) + 16 = 122\ g/mol$

$A.E = \frac{94}{122} \times 100\% = 77\%$

(c) $\sum FW = 7(12) + 8 + 4(16) = 156\ g/mol$

$A.E = \frac{94}{156} \times 100\% = 60\%$

Answer: Process b

Goal of a Chemical Process Engineer

- Find the optimal balance between maximizing **productivity** and **product quality**, while minimizing **waste**
- **How to measure waste?**
  - Yield vs Atomic energy
    - ✓ Atom economy is more useful than yield because it explicitly takes into account atoms that create a desired product versus those that create waste, *even if the process operates at maximum theoretical yield.*
    - ✓ Thus, whereas a yield calculation tells us how well an *already chosen* process operates, atom economy helps us decide which process (out of several possibilities) *should be chosen.*

Goal of a Chemical Process Engineer

- Find the optimal balance between maximizing **productivity** and **product quality**, while minimizing **waste**
- **How to measure product quality?**
  - Purity

$$\text{Purity} = 100 \text{ x } \frac{\text{g product}}{\sum \text{g product impurities}}$$

- **Other goals for the chemical process engineer:**
  - Scalability
  - Process safety

Goal of a Chemical Process Engineer

- **How do chemical process engineers achieve these goals?**

  Very generally speaking, in four steps:

  1. Choose a chemical process (from different options identified in collaboration with a chemist)
  2. Choose a process configuration
  3. Establish, through a combination of experiment and theory, quantitative relationships between process variables they care about (dependent variables) and those they get to choose (independent variables).
  4. Use these relationships to estimate values of the independent variables at which they can achieve their target volumetric productivity, yield, and product quality (this is dictated by practical issues such as market needs, supply chain issues, etc.)

Exercise 1

Acrylonitrile, an important building block of many different plastics, is produced by the reaction of propylene, ammonia, and oxygen:

$$C_3H_6 + NH_3 + O_2 \rightarrow C_3H_3N + 3H_2O$$

a. The propylene, being the most expensive reactant, is usually the limiting reagent. If the reaction is performed in batch mode with 1.2 equivalents of ammonia and oxygen, calculate the maximum theoretical yield of acrylonitrile per kg propylene used. List all waste products and the quantities in which they are produced.

b. Calculate the atom economy of the above acrylonitrile-producing reaction.