Unit 3: Fundamentals of material balances on reactive processes

Reminders

- Homework 2B is due on September 20
- AIChE panel in class on Friday, September 20
- On Monday, September 23: No in-person class (video will be posted on Canvas) and no office hours

Announcements

- Quiz 1 will be in class on Friday, September 27
- HW 3A will be due on Friday, September 27 (short)

Office Hours:

Posted here and on the Canvas homepage.

Day	Time	Location	Personnel
Monday	4 – 5PM	AW Smith 147	Duval
Tuesday	1 -2 PM	AW Smith, 152	TA
Wednesday	3:30 – 4:30 PM	AW Smith, 147	Duval
Thursday	2:30 – 3:30 PM	AW Smith 152	TA

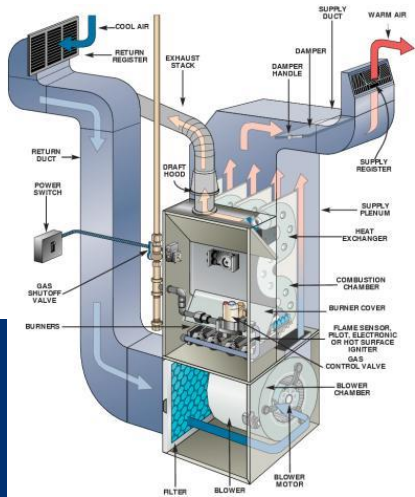
Helpful sections of the book: Chapter 4 (Sections 4.6- 4.10)

Learning Objectives

- After today's class students should be able to:
  - Define and calculate:
    - Yield
    - Selectivity
    - Fractional conversion
    - Extent of reaction
  - Write material balances using the extent of reaction method

Examples of Reactive Processes

- Manufacturing fertilizers
  - $2NH_3 + CO_2 \rightarrow NH_2CONH_2 + H_2O$
- Fermentation (brewing beer or wine)
  - $C_6H_{12}O_6 \rightarrow C_2H_5OH + 2CO_2$
- Natural gas combustion (heating your home)
  - $CH_4 + 2O_2 \rightarrow 2H_2O + CO_2$



Stoichiometry

- Stoichiometry is the theory of proportions in which chemical species combine with each other.

$$2H_2 + O_2 \rightarrow 2H_2O$$

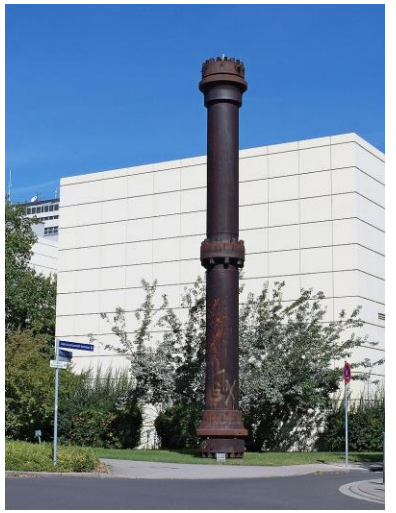
For any reaction, we should be able to answer:

- Is the stoichiometric equation balanced?
- What are the stoichiometric coefficients?
- What are the stoichiometric ratios?

Stoichiometry exercise

The Haber process is used for the industrial production of ammonia. The reaction combines nitrogen with hydrogen.

- Write a balanced chemical reaction.
- If 100 mol of nitrogen is fed to the reactor, how many mol of ammonia are produced?



Steel reactor from 1920s

More jargon

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

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

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

More jargon

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

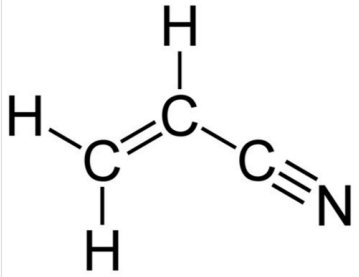
- Excess reactant
  - A reactant that is present in more than its stoichiometric proportion relative to every other reactant
- Fractional conversion
  - Ratio of (moles reacted)/(moles fed) for a given reactant

Even more jargon

- Extent of reaction (extent of conversion)

What do these things all have in common?

They all used acrylonitrile as a precursor!



Copolymers of acrylonitrile, styrene and butadiene

Carbon fibers come from poly(acrylonitrile) fibers

“acrylic” on clothing tags

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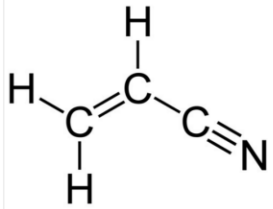

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New jargon for reactive processes with recycle

- Single-pass conversion
  - Fractional conversion of the reactor
- Overall conversion
  - Fractional conversion of the whole process

New jargon for systems with multiple chemical reactions

- Selectivity
  - $$\frac{moles\ of\ desired\ product}{moles\ of\ undesired\ product(s)}$$
- Yield
  - $$\frac{moles\ of\ desired\ product}{theoretical\ moles\ of\ desired\ product}$$
  - **Theoretical moles:** if no side reaction occurred, what is the maximum moles that could be produced in the given reactor

Production of Ethylene Oxide

ethylene oxide