CAREER FAIR WEEK

- BYU Bridge
- Info Sessions
- AIChE Activities

Strategy to Finish Ch. 4

- Mon (2/6) – 4.6 Chemical Reaction Terminology
- Wed (2/8) – 4.7 Balances on Process with Reactions, including DOF
- Thurs (2/9) – STEM CAREER FAIR
- Fri (2/10) – 4.7 Practice balances w/reactions
- Mon (2/13) – 4.8 Combustion

Word to the Wise

- Balances with chemical reaction are:
  - Easy!
  - Most missed competency on the L3 exam!

Non-Stoichiometric

- $N_2 + 3H_2 \rightarrow 2NH_3$
- Occurs quite a bit!
- Limiting reactant – whichever reactant will be consumed first!
  - If we start with 1 mole $N_2$, 2 moles $H_2$, then $H_2$ is the limiting reactant
  - If the 2 moles of $H_2$ are consumed, there will still be $N_2$ left!
- Excess reactant – whichever reactant would be left over after consuming the limiting reactant
  - In the example above, $N_2$ is the excess reactant

Stoichiometric

(I shouldn’t have to review this)

- $N_2 + 3H_2 \rightarrow 2NH_3$
- Stoichiometric coefficients ($v_i$)
  - Found in stoichiometric equation (numbers in front of species that balance the equation)
  - Negative for reactants, positive for products
  - $v_{N_2} = -1, v_{H_2} = -3, v_{NH_3} = 2$
- Stoichiometric ratio
  - Molar ratio in stoichiometric equation
  - The stoichiometric ratio here is $N_2/H_2 = 1/3$
  - If we actually have a system that has a 1:3 proportion, then we say it is in stoichiometric proportion

More Terms

(N2 + 3H2  → 2NH3)

- Stoichiometric Requirement
  - Given $x$ number of moles of one reactant, how many moles of the other reactant(s) are needed in stoichiometric proportion?
  - Given 2 moles of $N_2$, what is the stoichiometric requirement of $H_2$ to form $NH_3$? (6 moles)
- Percent Excess Suppose we have 2 moles $N_2$ and 7 moles $H_2$
  - There will be 1 mole of $H_2$ left after complete reaction
  - % excess = $\frac{(n_{i,0} - n_{i, stoich})}{n_{i, stoich}}$ • $(7-6)/6$ in this case = 1/6, or 16.7% excess $H_2$
Fractional Conversion

- \( f_i \) in our text, \( X_i \) in most others
  - Relative amount of reactant converted
    \[ \frac{n_{reacted}}{n_{fed}} \]
  - \( f_i \) (or \( X_i \)) = \( \frac{n_i - n_{i0}}{n_{i0}} = 1 - \frac{n_i}{n_{i0}} \)
- Start with 3 moles \( H_2 \), end with 0.3 moles \( H_2 \), then
  \( f_{H_2} = \frac{3 - 0.3}{3} = 0.9 \), or 90% conversion

Extent of Reaction

- \( \xi \), pronounced ksee
  - Moles reacted, normalized to stoichiometric equation
    \[ n_i = n_{i0} + \xi v_i \]
    or
    \[ \xi = \frac{n_i - n_{i0}}{v_i} \]
  - Note that \( v_i \) is negative for a reactant, positive for a product
  - \( \xi \) has units of moles
  - One value of \( \xi \) for each reaction (not one per species)

Example

- Start with 3 moles \( H_2 \) and 1.5 moles \( N_2 \)
  - 0.3 moles of \( H_2 \) are left after rxn (measured)
  - \( \xi = \frac{n_i - n_{i0}}{v_i} = \frac{0.9}{2} = 0.45 \) moles
  - \( n_{NH_3} = n_{i0} + \xi v_i = 0 + 0.9 \times 2 = 1.8 \) moles
  - Also, \( n_{N_2} = 1.5 + (0.9) \times (-1) = 0.6 \) moles
  - Note that \( \xi \) does not change with species, but there is one \( \xi \) for each reaction

Practice

- \( C_3H_8 + \frac{7}{2} O_2 \rightarrow 3 CO + 4 H_2O \)
- Start with 2 moles propane, 10 moles \( O_2 \)
- Limiting reactant: propane
- %Excess of excess reactant:
  \[ \frac{(10 - 7)}{7} \times 100 = 42.8\% \]

If 1.5 moles of propane react,
  - Fractional conversion \( f_{C_3H_8} = \frac{2 - 0.5}{2} = 75\% \)
  - Extent of reaction \( \xi = \frac{0.5 - 3}{(1)\times(1)} = 1.5 \) moles
  - \( n_{CO} = 10 \times (1.5) \times (-7/2) = 4.75 \) moles
  - \( n_{H_2O} = 0 + 1.5 \times 3 = 4.5 \) moles
  - \( n_{H_2O} = 0 + 1.5 \times 4 = 6.0 \) moles

Multiple Reactions

- Use \( \xi \)'s in mole balance for each species
  - \( C_2H_6 + \frac{5}{2} O_2 \rightarrow 2CO + 3H_2O \)
  - \( CO + \frac{1}{2} O_2 \rightarrow CO_2 \)
  - There must be a different extent of reaction for each reaction!
    - \( \xi_1 \) for reaction 1
    - \( \xi_2 \) for reaction 2
  - In general, for \( j \) reactions (\( i \) is for species)
    \[ n_i = n_{i0} + \sum_j v_{ij} \xi_j \]
Multiple Reactions

Use \( \xi \) in mole balance for each species

\[
\begin{align*}
\text{C}_2\text{H}_6 + \frac{5}{2} \text{O}_2 & \rightarrow 2\text{CO} + 3\text{H}_2\text{O} \\
\text{CO} + \frac{1}{2} \text{O}_2 & \rightarrow \text{CO}_2
\end{align*}
\]

Mole balances:

\[
\begin{align*}
\text{n}_{\text{C}_2\text{H}_6} &= n_{\text{C}_2\text{H}_6,0} - \xi_1 \\
\text{n}_{\text{O}_2} &= n_{\text{O}_2,0} - \frac{5}{2} \xi_1 - \frac{5}{2} \xi_2 \\
\text{n}_{\text{CO}} &= n_{\text{CO},0} + 2 \xi_1 - \xi_2 \\
\text{n}_{\text{H}_2\text{O}} &= n_{\text{H}_2\text{O},0} + 3 \xi_1 \\
\text{n}_{\text{CO}_2} &= n_{\text{CO}_2,0} + \xi_2
\end{align*}
\]

Yield & Selectivity

• These both have to do with multiple products, only one of which is most desired
  
  ★ Yield = (moles of desired product)/ (max possible moles at complete conversion)
  
  • Selectivity = (moles desired product)/(sum of undesired products)
    – There are lots of ways to define selectivity
    – Often it is where the carbon goes, and we ignore H\(_2\) as a product when calculating selectivity

Practice

\[
\begin{align*}
\text{C}_2\text{H}_6 & \rightarrow \text{C}_2\text{H}_4 + \text{H}_2 \\
\text{C}_2\text{H}_4 + \text{H}_2 & \rightarrow 2\text{CH}_4 \\
\text{C}_2\text{H}_4 + \text{C}_2\text{H}_6 & \rightarrow \text{C}_3\text{H}_6 + \text{CH}_4
\end{align*}
\]

Start with 100 moles of C\(_2\)H\(_6\)

After reaction, we have:

65 mols C\(_2\)H\(_4\)

15 mols C\(_2\)H\(_6\)

60 mols H\(_2\)

25 mols CH\(_4\)

5 mols C\(_3\)H\(_6\)

• Find yield and selectivity if C\(_2\)H\(_4\) is the desired product
• Find \( \xi_1, \xi_2, \) and \( \xi_3 \)

Answers (fill-in)

• Yield\(_{\text{C}_2\text{H}_4} = 65/100 = 65\%\)
• Selectivity = 65/(25 + 5) = 2.2
• Set up each mole balance

\[
\begin{align*}
\text{n}_{\text{C}_2\text{H}_6} &= 15 \text{ moles} = n_{\text{C}_2\text{H}_6,0} - \xi_1 - \xi_3 \\
\text{n}_{\text{C}_2\text{H}_4} &= 65 \text{ moles} = 0 + \xi_1 - \xi_3 \\
\text{n}_{\text{H}_2} &= 60 \text{ mols} = 0 + \xi_2 - \xi_3 \\
\text{n}_{\text{C}_3\text{H}_6} &= 5 \text{ mols} = 0 + \xi_3 \\
\end{align*}
\]

So,…

\[
\begin{align*}
\xi_3 &= 5 \text{ mols} \\
\xi_1 &= 65 + 5 = 70 \text{ mols (from C}_2\text{H}_4 \text{ balance)} \\
\xi_2 &= 70 - 60 = 10 \text{ mols (from H}_2 \text{ balance)}
\end{align*}
\]

Answers

• Yield\(_{\text{C}_2\text{H}_4} = 65/100 = 65\%\)
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\end{align*}
\]

Example:

\[
\text{CO}_2 + 3 \text{H}_2 \rightarrow \text{CH}_3\text{OH} + \text{H}_2\text{O}
\]

Suppose you had 100 mol of CO\(_2\) and 250 mol of H\(_2\), find limiting reactant and % excess of other reactant

• Limiting reactant = H\(_2\)
• % Excess CO\(_2\) = (100-250/3)/(250/3) = 20\%

Suppose 80 mol of CH\(_3\)OH was formed, find \( \xi \) and \( f_{\text{H}_2} \).

\[
\begin{align*}
\xi &= n_{\text{CH}_3\text{OH}} - 0/1 = 80 \text{ mol (also = n}_{\text{H}_2} \\
n_{\text{CO}_2} &= 100 \text{ mol} - (1)(\xi) = 20 \text{ mol} \\
n_{\text{H}_2} &= 250 \text{ mol} - (3)(\xi) = 10 \text{ mol} \\
f_{\text{H}_2} &= X_{\text{H}_2} = (250 - 10)/250 = 1 - 10/250 = 0.96 \ (i.e., \ 96\%)
\end{align*}
\]
Equilibrium Example
(page 122 in book)

CO + H₂O = CO₂ + H₂,
start with 1 mol CO, 2 mol H₂O

\[ \frac{y_{CO}}{y_{H₂O}} = \frac{K_v}{y_{CO}y_{H₂O}} \]

\[ \begin{align*}
    n_{CO} &= 1.0 - \xi \\
    n_{H₂O} &= 2.0 - \xi \\
    n_{CO₂} &= \xi \\
    n_{H₂} &= \xi \\
    n_{tot} &= 3.0
\end{align*} \]

Strategy:
- Plug expressions for \( y_i \) into equilibrium expression
- Solve for \( \xi \) (quadratic eqn. or use solver)
- Calculate final moles of each species from \( \xi \)
- Calculate \( f_{CO} \)