



# Class 12



# Strategy to Finish Ch. 4

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Mon (2/2) – 4.6

Wed (2/4) – 4.7, but not DOF

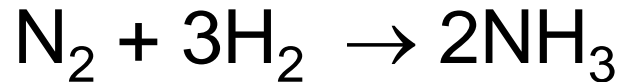
Thur (2/5) – Dean's lecture

Fri (2/6) – 4.7 DOF

Mon (2/9) – 4.8 Combustion

# Stoichiometric

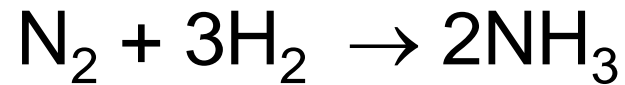
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- **Stoichiometric coefficients** ( $v_i$ )
  - Found in stoichiometric equation (numbers in front of species that balance the equation)
  - Negative for reactants, positive for products
  - $v_{\text{N}_2} = -1$ ,  $v_{\text{H}_2} = -3$ ,  $v_{\text{NH}_3} = 2$
- **Stoichiometric ratio**
  - Molar ratio in stoichiometric equation
    - The stoichiometric ratio here is  $\text{N}_2/\text{H}_2 = 1:3$
  - If we actually have a system that has a 1:3 proportion, then we say it is in **stoichiometric proportion**

# Non-Stoichiometric

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- Occurs quite a bit!
- **Limiting reactant** – whichever reactant will be consumed first!
  - If we start with 1 mole  $\text{N}_2$ , 2 moles  $\text{H}_2$ , then  $\text{H}_2$  is the limiting reactant
    - If the 2 moles of  $\text{H}_2$  are consumed, there will still be  $\text{N}_2$  left!
- **Excess reactant** – whichever reactant will be left over
  - In the example above,  $\text{N}_2$  is the excess reactant

# More Terms

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- **Stoichiometric Requirement**

- Given x number of moles, 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 moles of  $H_2$  left after complete reaction

- % excess =  $(n_{i,0} - n_{i, \text{stoich}})/n_{i, \text{stoich}}$

- =  $(7-6)/6$  in this case =  $1/6$ , or 16.7% excess  $H_2$

# Reaction-Related Terms

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- **Fractional Conversion**

( $f_i$  in our text,  $X_i$  in others)

– Relative amount of reactant converted (=  $n_{\text{reacted}}/n_{\text{fed}}$ )

–  $f_i$  (or  $X_i$ ) =  $(n_{i0} - n_i)/n_{i0} = 1 - n_i/n_{i0}$

- Start with 3 moles  $\text{H}_2$ , end with 0.3 moles  $\text{H}_2$ , then  $f_{\text{H}_2} = (3 - 0.3)/3 = 0.9$ , or 90% conversion

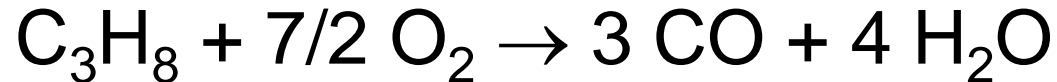
# Reaction-Related Terms

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- **Extent of Reaction** ( $\xi$ , pronounced ksee)
  - Amount of reacted, normalized to stoichiometric equation
  - $n_i = n_{i0} + \xi v_i$  or  $\xi = (n_i - n_{i0})/v_i$
  - note that  $v_i$  is negative for a reactant, positive for a product
  - Example
    - Start with 3 moles  $H_2$ , 1.5 moles  $N_2$ , 0.3 moles of  $H_2$  are left after rxn
    - $\xi = (0.3 - 3) / (-3) = 2.7/3 = 0.9$  moles
    - So  $n_{NH_3} = 0 + (0.9) \cdot (2) = 1.8$  moles
    - Also,  $n_{N_2} = 1.5 + (0.9) \cdot (-1) = 0.6$  moles
  - note that there is one  $\xi$  for each reaction

# Practice (fill-in)

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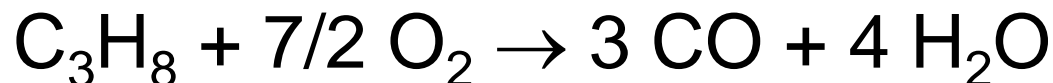
- Start with 2 moles propane, 10 moles  $\text{O}_2$
- Limiting reactant:
- %Excess of excess reactant:

If 1.5 moles of propane react,

- Fractional conversion (f) =
- Extent of reaction ( $\xi$ ) =
- $n_{\text{O}_2}$  =
- $n_{\text{CO}}$  =
- $n_{\text{H}_2\text{O}}$  =

# Practice

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- Start with 2 moles propane, 10 moles  $\text{O}_2$
- Limiting reactant: propane
- %Excess of excess reactant:

$$(10 - 7)/7 = 3/7 = 42.8\%$$

If 1.5 moles of propane react,

- Fractional conversion (f) =  $(2 - 0.5)/2 = 75\%$
- Extent of reaction ( $\xi$ ) =  $(0.5 - 2)/(-1) = 1.5$  moles
- $n_{\text{O}_2} = 10 + (1.5) \cdot (-7/2) = 4.75$  moles
- $n_{\text{CO}} = 0 + 1.5 \cdot 3 = 4.5$  moles
- $n_{\text{H}_2\text{O}} = 0 + 1.5 \cdot 4 = 6.0$  moles

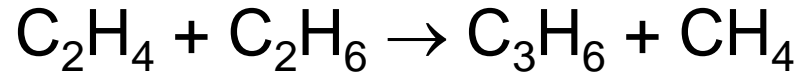
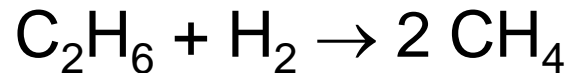
# Yield & Selectivity

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- 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)

# Practice

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Start with 100 moles of  $\text{C}_2\text{H}_6$

After reaction, we have:

65 mols  $\text{C}_2\text{H}_4$

15 mols  $\text{C}_2\text{H}_6$

60 mols  $\text{H}_2$

25 mols  $\text{CH}_4$

5 mols  $\text{C}_3\text{H}_6$

- Find yield and selectivity if  $\text{C}_2\text{H}_4$  is the desired product
- Find  $\xi_1$ ,  $\xi_2$ , and  $\xi_3$

# Answers (fill-in)

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- Yield<sub>C<sub>2</sub>H<sub>4</sub></sub> = 65/100 = 65%
- Selectivity = 65/(25 + 5) = 2.2
- Set up each mole balance
  - $n_{\text{C}_2\text{H}_6} = 15 \text{ moles} = n_{\text{C}_2\text{H}_6,0} - \xi_1 - \xi_2 - \xi_3$
  - $n_{\text{C}_2\text{H}_4} = 65 \text{ moles} =$
  - $n_{\text{H}_2} = 60 \text{ moles} =$
  - $n_{\text{C}_3\text{H}_6} = 5 \text{ mols} =$

So.....

$$\xi_3 =$$

$$\xi_1 =$$

$$\xi_2 =$$

# Answers

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- Yield<sub>C<sub>2</sub>H<sub>4</sub></sub> = 65/100 = 65%
- Selectivity = 65/(25 + 5) = 2.2
- Set up each mole balance
$$n_{\text{C}_2\text{H}_6} = 15 \text{ moles} = n_{\text{C}_2\text{H}_6,0} - \xi_1 - \xi_2 - \xi_3$$
$$n_{\text{C}_2\text{H}_4} = 65 \text{ moles} = 0 + \xi_1 - \xi_3$$
$$n_{\text{H}_2} = 60 \text{ moles} = 0 + \xi_1 - \xi_2$$
$$n_{\text{C}_3\text{H}_6} = 5 \text{ mols} = 0 + \xi_3$$

So.....

$$\xi_3 = 5 \text{ mols}$$

$$\xi_1 = 65 + 5 = 70 \text{ mols} \quad (\text{from C}_2\text{H}_4 \text{ balance})$$

$$\xi_2 = 70 - 60 = 10 \text{ mols} \quad (\text{from H}_2 \text{ balance})$$

## Example:



Suppose you had 100 mol of  $\text{CO}_2$  and 250 mol of  $\text{H}_2$ ,  
find limiting reactant and % excess of other reactant

- Limiting reactant =  $\text{H}_2$
- % Excess  $\text{CO}_2 = (100 - 250/3)/(250/3) = 20\%$

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

- $n_{\text{CH}_3\text{OH}} = (1) \cdot (\xi) = 80 \text{ mol} (= n_{\text{H}_2\text{O}})$
- $n_{\text{CO}_2} = 100 \text{ mol} - (1) \cdot (\xi) = 20 \text{ mol}$
- $n_{\text{H}_2} = 250 \text{ mol} - (3) \cdot (\xi) = 10 \text{ mol}$
- $f_{\text{H}_2} = (250 - 10)/250 = 1 - 10/250 = 0.96$  (i.e., 96%)