CHEMICAL CALCULATIONS CONTINUED: REACTIONS

- Chemical reactions proceed on an ATOMIC basis, NOT a mass basis!

- To calculate with chemical reactions (i.e. use chemical equations), we need everything in terms of ATOMS ... which means MOLES of atoms

$$2\,Al(s) + 3\,Br_2(l) \longrightarrow 2\,AlBr_3(s)$$

coefficients are in terms of atoms and molecules!

2 atoms Al = 3 molecules Br_2 = 2 formula units $AlBr_3$

2 mol Al = 3 mol Br_2 = 2 mol $AlBr_3$

- To do chemical calculations, we need to:
    - Relate the amount of substance we know (mass or volume) to a number of moles
    - Relate the moles of one substance to the moles of another using the equation
    - Convert the moles of the new substance to mass or volume as desired

$$2Al(s) + 3Br_2(l) \longrightarrow 2AlBr_3(s)$$

* Given that we have 25.0 g of liquid bromine, how many grams of aluminum would we need to react away all of the bromine? How many grams of aluminum bromide would be produced?

(1) Convert grams of bromine to moles: Need formula weight

$$Br_2: \frac{2 \times 79.90}{159.80}$$

$$159.80\,g\,Br_2 = 1\,mol\,Br_2$$

$$25.0\,g\,Br_2 \times \frac{1\,mol\,Br_2}{159.80\,g\,Br_2} = 0.15645\,mol\,Br_2$$

(2) Use the chemical equation to relate moles of bromine to moles of aluminum

$$2\,mol\,Al = 3\,mol\,Br_2$$

$$0.15645\,mol\,Br_2 \times \frac{2\,mol\,Al}{3\,mol\,Br_2} = 0.10430\,mol\,Al$$

(3) Convert moles aluminum to mass: Need formula weight

$$Al: 26.98$$

$$26.98\,g\,Al = 1\,mol\,Al$$

$$0.10430\,mol\,Al \times \frac{26.98\,g\,Al}{1\,mol\,Al} = \boxed{2.81\,g\,Al}$$

You can combine all three steps on one line if you like!

$$25.0\,g\,Br_2 \times \frac{1\,mol\,Br_2}{159.80\,g\,Br_2} \times \frac{2\,mol\,Al}{3\,mol\,Br_2} \times \frac{26.98\,g\,Al}{1\,mol\,Al} = \boxed{2.81\,g\,Al}$$

1 2 3

$$\begin{array}{r} 25.0\,g\,Br_2 \\ +\ 2.81\,g\,Al \\ \hline 27.8\,g\,AlBr_3 \end{array}$$

But ...
...what would you have done to calculate the mass of aluminum bromide IF you had NOT been asked to calculate the mass of aluminum FIRST?

$$25.0\,g\,Br_2 \times \frac{1\,mol\,Br_2}{159.80\,g\,Br_2} \times \frac{2\,mol\,AlBr_3}{3\,mol\,Br_2} \times \frac{266.694\,g\,AlBr_3}{1\,mol\,AlBr_3} = 27.8\,g$$

1 convert mass bromine to moles

2 convert moles bromine to moles aluminum bromide

3 convert moles aluminum bromide to mass

Example:
How many milliliters of 6.00M hydrochloric acid is needed to completely react with 25.0 g of sodium carbonate?

$$2HCl(aq) + Na_2CO_3(s) \longrightarrow H_2O(l) + CO_2(g) + 2NaCl(aq)$$

1 - Convert mass of sodium carbonate to moles using formula weight
2 - Convert moles of sodium carbonate to moles hydrochloric acid using chemical equation
3 - Convert moles of hydrochloric acid to volume using concentration (M = moles/L)

- Convert mass of sodium carbonate to moles using formula weight

Na_2CO_3: Na : 2 x 22.99
C : 1 x 12.01
O : 3 x 16.00
105.99

$105.99\,g\ Na_2CO_3 = 1\ mol\ Na_2CO_3$

$$25.0\,g\ Na_2CO_3 \times \frac{1\ mol\ Na_2CO_3}{105.99\,g\ Na_2CO_3} = 0.23587\ mol\ Na_2CO_3$$

Example:

How many milliliters of 6.00M hydrochloric acid is needed to completely react with 25.0 g of sodium carbonate?

$$2HCl(aq) + Na_2CO_3(s) \longrightarrow H_2O(l) + CO_2(g) + 2NaCl(aq)$$

- Convert moles of sodium carbonate to moles hydrochloric acid using chemical equation

$$2 \text{ mol } HCl = 1 \text{ mol } Na_2CO_3$$

$$0.23587 \text{ mol } Na_2CO_3 \times \frac{2 \text{ mol } HCl}{1 \text{ mol } Na_2CO_3} = 0.47174 \text{ mol } HCl$$

- Convert moles of hydrochloric acid to volume using concentration (M = moles/L)

$$6 \text{ mol } HCl = 1 L$$

$$0.47174 \text{ mol } HCl \times \frac{1 L}{6 \text{ mol } HCl} = 0.0786 L \text{ of } HCl$$

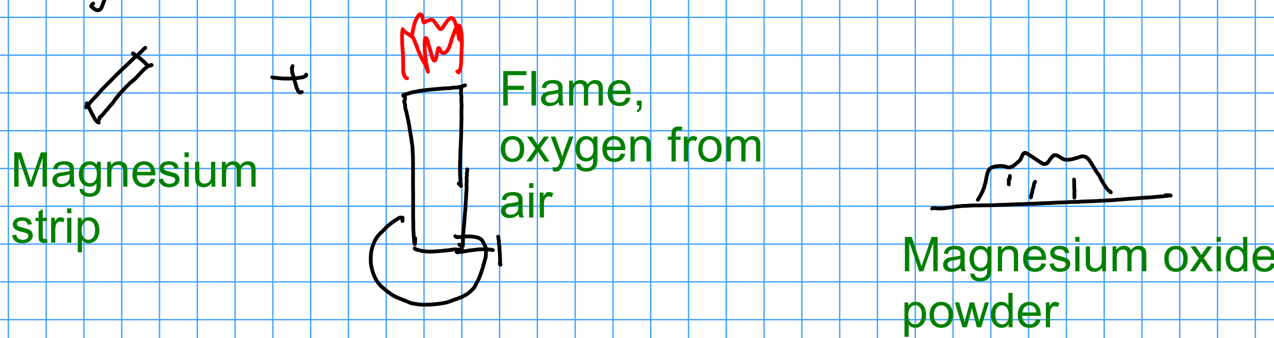
$$mL = 10^{-3} L$$ Convert liters to milliliters!

$$0.0786 L \times \frac{mL}{10^{-3} L} = \boxed{78.6 \text{ mL of } 6.00M \text{ } HCl}$$

CONCEPT OF LIMITING REACTANT

- When does a chemical reaction STOP?

$$2Mg(s) + O_2(g) \xrightarrow{\Delta} 2MgO(s)$$



- When does this reaction stop? When burned in open air, this reaction stops when all the MAGNESIUM STRIP is gone. We say that the magnesium is LIMITING.

- This reaction is controlled by the amount of available magnesium

- At the end of a chemical reaction, the LIMITING REACTANT will be completely consumed, but there may be amount of OTHER reactants remaining. We do chemical calculations in part to minimize these "leftovers".

These are often called "excess" reactants, or reactants present "in excess"

LIMITING REACTANT CALCULATIONS

- To find the limiting reactant, calculate how much product would be produced from ALL given reactants. Whichever produces the SMALLEST amouht of product is the limiting reactant, and the smallest anount of product is the actual amount of product produced.

Example:

$$\underset{56.08}{CaO(s)} + \underset{12.01}{3C(s)} \xrightarrow{\Delta} \underset{64.10}{CaC_2(s)} + CO(g)$$

If you start with 100. g of each reactant, how much calcium carbide would be produced?

56.08 g CaO = 1 mol CaO   64.10 g CaC_2 = 1 mol CaC_2

1 mol CaO = 1 mol CaC_2

$$100.\ g\ CaO \times \frac{1\ mol\ CaO}{56.08\ g\ CaO} \times \frac{1\ mol\ CaC_2}{1\ mol\ CaO} \times \frac{64.10\ g\ CaC_2}{1\ mol\ CaC_2} = \boxed{114\ g\ CaC_2}$$

12.01 g C = 1 mol C   64.10 g CaC_2 = 1 mol CaC_2 3 mol C = 1 mol CaC_2

$$100.\ g\ C \times \frac{1\ mol\ C}{12.01\ g\ C} \times \frac{1\ mol\ CaC_2}{3\ mol\ C} \times \frac{64.10\ g\ CaC_2}{1\ mol\ CaC_2} = \boxed{178\ g\ CaC_2}$$

114g of calcium carbide are produced. Calcium oxide is limiting, and the reaction stops when all 100g of calcium oxide are gone! (There will be leftover carbon at the end of this reaction!)

PERCENT YIELD

- Chemical reactions do not always go to completion! Things may happen that prevent the conversion of reactants to the desired/expected product!

1 SIDE REACTIONS:

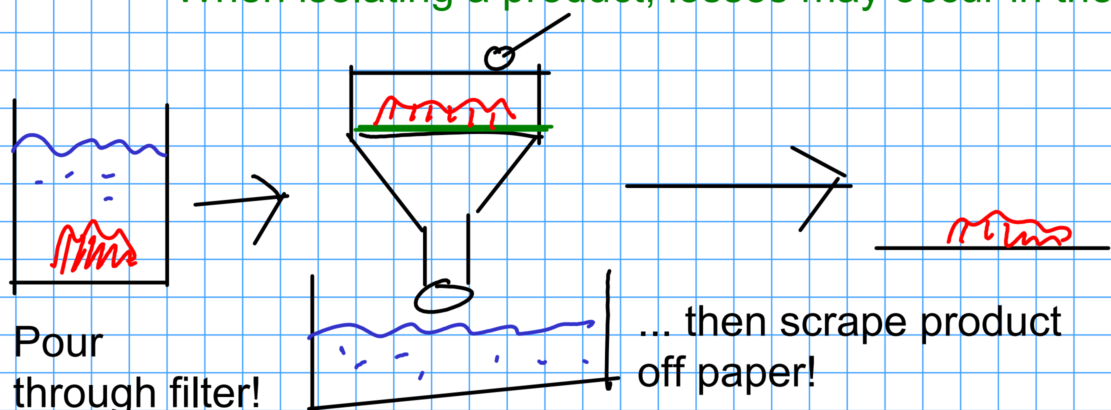
$C + O_2 \longrightarrow CO_2$ | This reaction occurs when there is a large amount of oxygen available

$2C + O_2 \longrightarrow 2CO$ | ... while this reaction is more favorable in low-oxygen environments!

... so in a low-oxygen environment, you may produce less carbon dioxide than expected!

2 TRANSFER AND OTHER LOSSES

- When isolating a product, losses may occur in the process. Example: filtering



Durning each step of this process, some amount of product loss will occur!

3 EQUILIBRIUM

- Reactions may reach an equilbrium between prodcuts and reactants. We'll talk more about this in CHM 111. The net results is that the reaction will appear to stop before all reactants have been consumed!

- All of these factors cause a chemical reaction to produce LESS product than calculated. For many reactions, this difference isn't significant. But for others, we need to report the PERCENT YIELD.

Determined EXPERIMENTALLY!

$$\text{PERCENT YIELD} = \frac{\text{ACTUAL YIELD}}{\text{THEORETICAL YIELD}} \times 100\%$$

Calculated based on the limiting reactant. (The chemical calculations you've done up to now have been theoretical yields!)

... the percent yield of a reaction can never be greater than 100% due to conservation of mass! If you determine that a percent yield is greater than 100%, then you've made a mistake somewhere - either in a calculation or in the experiment itself!

78.114 g/mol   123.111 g/mol

22.4 g   31.6 g ACTUAL

$$C_6H_6 + HNO_3 \longrightarrow C_6H_5NO_2 + H_2O$$

benzene   nitric acid   nitrobenzene

22.4 grams of benzene are reacted with excess nitric acid. If 31.6 grams of nitrobenzene are collected from the reaction, what is the percent yield?

$$\%Y = \frac{\text{actual}}{\text{theoretical}} \times 100\%$$

CALCULATE the amount of nitrobenzene that would form if ALL the benzene reacts.

78.114 g b = 1 mol b | 1 mol b = 1 mol nb | 123.111 g nb = 1 mol nb

$$22.4\,\cancel{g\,b} \times \frac{1\,\cancel{mol\,b}}{78.114\,\cancel{g\,b}} \times \frac{1\,mol\,nb}{1\,\cancel{mol\,b}} \times \frac{123.111\,g\,nb}{1\,mol\,nb} = 35.3\,g\,nb$$

THEORETICAL yield of nitrobenzene

$$\%\,Yield = \frac{31.6\,g\,nb}{35.3\,g\,nb} \times 100\% = \boxed{89.5\%}$$

$$\overset{42.081\ g/mol}{4\,C_3H_6} + 6\,NO \longrightarrow \overset{53.064\ g/mol}{4\,C_3H_3N} + 6\,H_2O + N_2$$

propylene — acrylonitrile

Calculate how many grams of acrylonitrile could be obtained from 651 kg of propylene, assuming there is excess NO present.

(651000 g)

42.081 g pp = 1 mol pp | 4 mol pp = 4 mol an

53.064 g an = 1 mol an

$$651000\,\cancel{g\ pp} \times \frac{1\,\cancel{mol\ pp}}{42.081\,\cancel{g\ pp}} \times \frac{4\,\cancel{mol}\ an}{4\,\cancel{mol\ pp}} \times \frac{53.064\ g\ an}{1\,\cancel{mol\ an}} =$$

$$\boxed{\begin{array}{c}821000\ g\ an \\ 8.21 \times 10^{5}\ g\ an\end{array}}$$

$$10\,FeSO_4 + 2\,KMnO_4 + 8\,H_2SO_4 \rightarrow 5\,Fe_2(SO_4)_3 + 2\,MnSO_4 + K_2SO_4 + 8\,H_2O$$

How many mL of 0.250M potassium permanganate are needed to react with 3.36 g of iron(II) sulfate?

$151.90\,g\ FeSO_4 = 1\ mol\ FeSO_4$ | $10\ mol\ FeSO_4 = 2\ mol\ KMnO_4$

$0.250\ mol\ KMnO_4 = 1\ L$

$$3.36\,g\ \cancel{FeSO_4} \times \frac{1\ \cancel{mol\ FeSO_4}}{151.90\,\cancel{g\ FeSO_4}} \times \frac{2\ \cancel{mol\ KMnO_4}}{10\ \cancel{mol\ FeSO_4}} \times \frac{1\ L}{0.250\ \cancel{mol\ KMnO_4}} =$$

$$mL = 10^{-3}\ L$$

$$0.0177\ L \times \frac{mL}{10^{-3}\ L} = \boxed{17.7\ mL\ of\ 0.250\ \underline{M}\ KMnO_4}$$