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

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

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?

① Convert grams of bromine to moles: Need formula weight $Br_2: \frac{2 \times 79.90}{159.80}$

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

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

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 $Al: 26.98$

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

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

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

① $154.80\,g\ Br_2 = mol\ Br_2$ ② $2\ mol\ Al = 3\ mol\ Br_2$ ③ $26.98\,g\ Al = mol\ Al$

$$25.0\,g\ Br_2 \times \underset{\textcircled{1}}{\frac{mol\ Br_2}{154.80\,g\ Br_2}} \times \underset{\textcircled{2}}{\frac{2\ mol\ Al}{3\ mol\ Br_2}} \times \underset{\textcircled{3}}{\frac{26.98\,g\ Al}{mol\ Al}} = \boxed{2.81\,g\ Al}$$

Things we can do:

If we have ...	... and we need ...	Use ...
MASS	MOLES	FORMULA WEIGHT
SOLUTION VOLUME	MOLES	MOLAR CONCETRATION (MOLARITY)
MOLES OF A	MOLES OF B	BALANCED CHEMICAL EQUATION

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 25.0 g sodium carbonate to moles. Use FORMULA WEIGHT.

2 - Convert moles sodium carbonate to moles HCl. Use CHEMICAL EQUATION.

3 - Convert moles HCl to solution volume. Use MOLARITY (6.00 M HCl)

---

① Na_2CO_3: Na − 2 x 22.99

C − 1 x 12.01

O − 3 x 16.00

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

$$25.0\,g\ Na_2CO_3 \times \frac{mol\ Na_2CO_3}{105.99\,g\ Na_2CO_3} = 0.2358713086\ mol\ Na_2CO_3$$

---

② $2\ mol\ HCl = mol\ Na_2CO_3$

$$0.2358713086\ mol\ Na_2CO_3 \times \frac{2\ mol\ HCl}{mol\ Na_2CO_3} = 0.4717426172\ mol\ HCl$$

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 25.0 g sodium carbonate to moles. Use FORMULA WEIGHT.
2 - Convert moles sodium carbonate to moles HCl. Use CHEMICAL EQUATION.
3 - Convert moles HCl to solution volume. Use MOLARITY (6.00 M HCl)

③ 6.00 mol HCl = L

$$0.4717426172 \text{ mol HCl} \times \frac{L}{6.00 \text{ mol HCl}} = 0.0786 \text{ L of } 6.00 \text{ M HCl}$$

Since the answer is in liters right now and the problem asks specifically for milliliters, we need to do a quick unit conversion.

$mL = 10^{-3} L$

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

$$4\,\underset{\text{propylene}}{\overset{42.081\text{ g/mol}}{C_3H_6}} + 6\,NO \longrightarrow 4\,\underset{\text{acrylonitrile}}{\overset{53,064\text{ g/mol}}{C_3H_3N}} + 6\,H_2O + N_2$$

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

---

1 - Convert 651 grams propylene to moles. Use FORMULA WEIGHT.
2 - Convert moles propylene to moles acrylonitrile. Use CHEMICAL EQUATION.
3 - Convert moles acrylonitrile to mass. Use FORMULA WEIGHT.

---

① $42.081\text{ g }C_3H_6 = \text{mol }C_3H_6$ ② $4\text{ mol }C_3H_6 = 4\text{ mol }C_3H_3N$

③ $53,064\text{ g }C_3H_3N = \text{mol }C_3H_3N$

$$651\text{ g }C_3H_6 \times \underset{①}{\frac{\text{mol }C_3H_6}{42,081\text{ g }C_3H_6}} \times \underset{②}{\frac{4\text{ mol }C_3H_3N}{4\text{ mol }C_3H_6}} \times \underset{③}{\frac{53.064\text{ g }C_3H_3N}{\text{mol }C_3H_3N}} = \boxed{821\text{ g }C_3H_3N}$$

$151.90\ g/mol$

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

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

---

1 - Convert 3.36 g iron(II) sulfate to moles. Use FORMULA WEIGHT.
2 - Convert moles iron(II) sulfate to moles potassium permangenate. Use CHEMICAL EQUATION
3 - Convert moles potassium permangenate to volume. Use MOLARITY (0.250 M)

---

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

③ $0.250\ mol\ KMnO_4 = L$

$$3.36\,g\ FeSO_4 \times \underset{\textcircled{1}}{\frac{mol\ FeSO_4}{151.90\,g\ FeSO_4}} \times \underset{\textcircled{2}}{\frac{2\ mol\ KMnO_4}{10\ mol\ FeSO_4}} \times \underset{\textcircled{3}}{\frac{L}{0.250\ mol\ KMnO_4}} = 0.0177\ L\ of\ 0.250\ m\ KMnO_4$$

Convert volume to mL because that unit was specified in the problem.

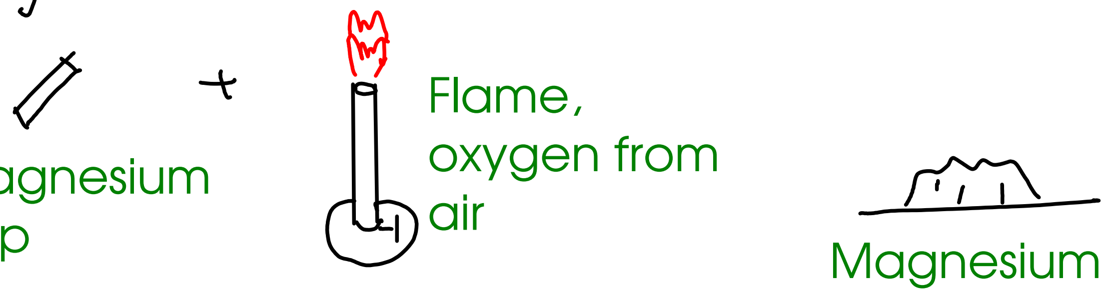
$mL = 10^{-3}\ L$

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

CONCEPT OF LIMITING REACTANT

- When does a chemical reaction STOP?

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



Magnesium strip

Flame, oxygen from air

Magnesium oxide powder

- 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: 56.08 12.01 64.10 <- Formula weights

$$\underline{CaO(s)} + 3\,\underline{C}(s) \xrightarrow{\Delta} CaC_2(s) + CO(g)$$

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

---

① 56.08g CaO = mol CaO ② mol CaO = mol CaC$_2$ ③ 64.10g CaC$_2$ = mol CaC$_2$

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

---

① 12.01g C = mol C ② 3 mol C = mol CaC$_2$ ③ 64.10g CaC$_2$ = mol CaC$_2$

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

Once the reaction produces 114 grams of calcium carbide, all the CaO has been used and the reaction must stop. There is C left over, but it has nothing to react with. We say that CaO is LIMITING and C is present IN EXCESS.

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:

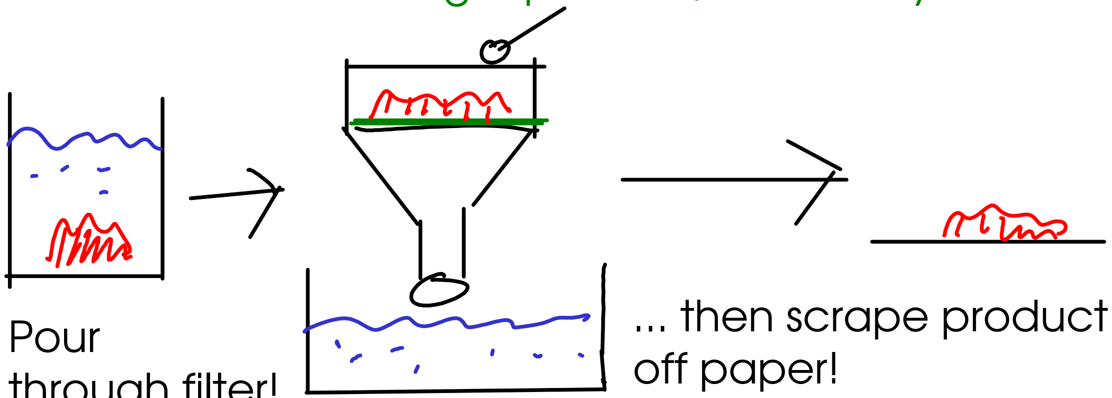
$C + O_2 \longrightarrow CO_2$ | This reaction occurs when there is a large amount of oxygen available

$2C + O_2 \longrightarrow 2CO$ | ... 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



Pour through filter!

... then scrape product off paper!

During 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!