Stoichiometry II

1. The use of a balanced chemical equation to calculate the quantities of the reactants and products of a reaction.

Abbreviations

1. Reaction = rxn
2. Solution = soln

2. A typical chemical equation:

$$CaCO_3(s) \longrightarrow CaO(s) + CO_2(g)$$

1. Read left to right
2. s, l, g, aq define physical states
3. proper chemical formulas or elemental symbols
4. Coefficients are the numbers that appear <u>before</u> the formula. There is a <u>1</u> in front of $CaCO_3$, CaO and CO_2. Coefficients are in units of <u>moles</u>.

(3) Law Conservation of Mass: A balanced equation has the same numbers and types of atoms on both sides of the arrow.

(4) Stoichiometry is based on the idea that a balanced equation relates the mole ratio in which reactants combine and the mole ratio in which the products are produced.

Example

$$\underline{1}CaCO_3 \longrightarrow \underline{1}CaO + \underline{1}CO_2$$

$\downarrow$ one particle — $\downarrow$ one particle — $\downarrow$ one particle

So it takes one particle of $CaCO_3$ to produce one particle each of CaO and CO_2.

$$CaCO_3 \longrightarrow CaO + CO_2$$

$\downarrow$ 1 mole $\downarrow$ 6×10^{23} — $\downarrow$ 1 mole $\downarrow$ 6×10^{23} — $\downarrow$ 1 mole $\downarrow$ 6×10^{23}

(5) Use the equation to do a basic calculation:

$$CaCO_3 \longrightarrow CaO + CO_2$$

	$CaCO_3$	CaO	CO_2	
Let's say we have	0.7 mole	0	0	Before any rxn takes place zero.
After rxn	0	0.7 mole	0.7 mole	After rxn
	Reactant is used up	Products produced in 1:1 ratio		

Use unit multiplier method for the same calculation:

$$\frac{0.7 \cancel{\text{mole}}\ \cancel{CaCO_3}}{1} \times \frac{1 \text{mole } CaO}{1 \cancel{\text{mole } CaCO_3}} = 0.7 \text{ mole } CaO$$

Coefficient from balanced equation

$$\frac{0.7 \cancel{\text{mole } CaCO_3}}{1} \times \frac{1 \text{mole } CO_2}{1 \cancel{\text{mole } CaCO_3}} = 0.7 \text{ mole } CO_2$$

(6) Use the equation for a more complicated calculation:

$$CaCO_3 \longrightarrow CaO + CO_2$$

$CaCO_3$: 9.7g

This time we're given mass. Step one is to convert mass to moles.

$$\frac{9.7g\ CaCO_3}{1} \times \frac{1\ \text{mole}}{100g\ CaCO_3} = 0.097\ \text{mole}\ CaCO_3$$

molecular weight $CaCO_3$

<u>Now</u>: ratio is 1:1:1

	$CaCO_3 \longrightarrow$	CaO +	CO_2
Before rxn	0.097 mole	0	0
After rxn	0	0.097 mole	0.097 mole

<u>unit multiplier</u>:

coefficient

a. $0.097\ \text{mole}\ CaCO_3 \times \frac{1\ \text{mole}\ CaO}{1\ \text{mole}\ CaCO_3} = 0.097\ \text{mole}\ CaO$

coefficient

b. $0.097\ \text{mole}\ CaCO_3\ \frac{1\ \text{mole}\ CO_2}{1\ \text{mole}\ CaCO_3} = 0.097\ \text{moles}\ CO_2$

To find the mass of CaO + CO_2 produced:

$$0.097 \cancel{\text{mole}}\ CaO \times \frac{56g\ CaO}{1 \cancel{\text{mole}}} = 5.43 \text{grams } CaO$$

molecular weight

$$0.097 \cancel{\text{moles}}\ CO_2 \times \frac{44g\ CO_2}{1 \cancel{\text{mole}}} = 4.27g\ CO_2$$

9.7g total mass

Remember this is the mass of $CaCO_3$ we started with.

(7)

Now lets work with an equation that is not 1:1:1.

1 : 3 : 2

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

0.36g — Start with mass

assume excess of H_2

0 ← Zero before rxn

Calculate the mass of NH_3 produced:

Step 1: convert mass N_2 to moles N_2

$$0.36g\ N_2 \times \frac{1 \text{mole } N_2}{28g\ N_2} = 0.013 \text{ mole } N_2$$

Step 2: convert moles N_2 to moles NH_3 produced.

$$0.013 \text{ mole } N_2 \times \frac{2 \text{ mole } NH_3}{1 \text{ mole } N_2} = 0.026 \text{ mole } NH_3$$

Step 3:

Now find mass of NH_3 produced.

$$0.026 \cancel{\text{mole}}\ NH_3 \times \frac{17\text{g } NH_3}{1 \cancel{\text{mole}}} = 0.442\text{g } NH_3$$

(8) Now we'll use the same equation to find the mass of H_2 required to react with N_2.

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

N_2	$3H_2$	$2NH_3$
0.013 mole	?	0.026 mole
0.36g		0.442g

$$0.013 \cancel{\text{mole}}\ N_2 \times \frac{3 \text{ mole } H_2}{1 \cancel{\text{mole } N_2}} = 0.039 \text{ mole } H_2$$

$$0.039 \text{ mole } H_2 \times \frac{2\text{g}}{1 \text{ mole}} = 0.078\text{g } H_2$$

9 Similar calculations can be used going in reverse. Let's say 12g NH_3 is produced in a rxn. Calculate mass N_2 and H_2 reacted.

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

? ? 12g

Step 1: convert 12g NH_3 to moles NH_3

$$12g\,NH_3 \times \frac{1\,mole}{17g\,NH_3} = 0.71\,moles\,NH_3$$

Step 2: use equation to find N_2 & H_2

$$0.71\,moles\,NH_3 \times \frac{1\,mole\,N_2}{2\,mole\,NH_3} \times \frac{28g\,N_2}{1\,mole} = 9.94g\,N_2$$

$$0.71\,moles\,NH_3 \times \frac{3\,mole\,H_2}{2\,mole\,NH_3} \times \frac{2g\,H_2}{1\,mole} = 2.13g\,H_2$$

(10) Theoretical yield

Theoretical yield represents the maximum amount of product in mass or moles that can be formed in a chemical rxn assuming that the rxn went to 100% completion.

In the previous example we determined that when 0.36g of N_2 reacted with an excess of H_2 that 0.442g NH_3 was produced. 0.442g NH_3 is the theoretical yield.

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

0.36g $\qquad$? ← Theo yield

$$0.013 \text{ mole } N_2 \times \frac{2NH_3}{1N_2} = 0.026 \text{ mole } NH_3 \times \frac{17g}{mole} = $$

$$= 0.442g$$

↑ Theo yield.

% yield

In order to evaluate a chemical rxn in practice we calculate % yield $= \frac{\text{actual yield}}{\text{Theo yield}} \times 100$

In the last rxn, if the actual yield was 0.39g then the % yield is: $\% = \frac{0.39}{0.442} \times 100 = 88.2\%$

The actual yield is the maximum product in mass or moles obtained when the rxn is carried out in the laboratory. The % yield is always smaller than 100% because no rxn is ever perfectly carried out by the chemist.

Limiting Reactant

In any chemical rxn where two or more reactants are combined by providing mass or mole amounts of all reactants at once, one of the reactants will run out bringing a halt to the rxn. The reactant that runs out is the limiting reactant.

Consider the following example: If we combine 100 cars with no tires with 350 tires we cannot produce 100 functioning cars. This is because for 100 cars we need 400 tires.

For 100 cars: $100 \text{ cars} \times \frac{4 \text{ tires}}{1 \text{ car}} = 400 \text{ tires needed}$

$350 \text{ tires} \times \frac{1 \text{ car}}{4 \text{ tires}} = 87.5 \text{ cars}$ or 87 complete cars.

The bottom line is that 13 cars will be left uncompleted. The tires are the limiting reactant.

Now let's consider a chemical example:

2g of N_2 is combined with 2g H_2 to produce ammonia (NH_3):

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

The goal: 1. calculate the limiting reactant
2. calculate theo yield of NH_3
3. calculate mass of the remaining reactant.

(A) First re-write information

$$\begin{array}{ccccc} N_2 & + & 3H_2 & \rightarrow & 2NH_3 \\ 2g & & 2g & & ? \end{array}$$

(B) Calculate theo yield of NH_3 using BOTH reactants

$$2g\ N_2 \times \frac{1\,mole}{28g} = 0.071428\,mole\,N_2 \times \frac{2NH_3}{1N_2} = 0.142857\,mole\,NH_3 \times 17g/mole = 2.43g\ NH_3$$

$$2g\ H_2 \times \frac{1\,mole}{2.016g} = 0.992063\,mole\,H_2 \times \frac{2NH_3}{3H_2} = 0.661375\,mole\,NH_3$$

(C) Evaluate which reactant produced less NH_3. This is the limiting reactant. Thus, the Limiting Reactant (LR) is N_2. Now multiply by Mm NH_3 to get the Theo yield: $0.142857\,mole\,NH_3 \times \frac{17g}{mole} = 2.43g\ NH_3$

(d) Now find mass remaining reactant. The main thing here to Know is that you must use the moles of the limiting reactant to first find the moles of the other reactant that were used in the rxn. Then this mass value is subtracted from the mass given.

we pull down the moles N_2:

$$0.071428 \text{ moles } N_2 \times \frac{3 H_2}{N_2} = 0.21428 \text{ moles } H_2 \times \frac{2.016g}{mole}$$

$$= 0.432g\ H_2$$

This is the mass of H_2 used up in the rxn when the 2g of N_2 reacts completely.

To find H_2 that remains behind:

$$\underset{\text{given}}{2g\,H_2} - \underset{\text{used}}{0.432g\,H_2} = \underset{\text{Remains unreacted}}{1.568g\,H_2}$$