Calculations from chemical equations

If you know the amount of any reactant or product involved in the reaction:

• you can calculate the amounts of all the other reactants and products that are consumed or produced in the reaction

$$C_3H_8(g) + 5 O_2(g) \longrightarrow 3 CO_2(g) + 4 H_2O(g)$$

BUT REMEMBER!

The coefficients in a chemical equation provide information ONLY about the proportions of MOLES of reactants and products

- given the number of moles of a reactant/product involved in a reaction, you CAN directly calculate the number of moles of other reactants and products consumed or produced in the reaction
- given the mass of a reactant/product involved in a reaction, you can NOT <u>directly</u> calculate the mass of other reactants and products consumed or produced in the reaction

Mole - mole calculations

Given: • A balanced chemical equation

• A known quantity of one of the reactants/product (in moles)

Calculate: The quantity of one of the other reactants/products (in moles)



Mole - mole calculations

Example:

How many moles of ammonia are produced from 8.00 mol of hydrogen reacting with nitrogen?

2 NH₃

Equation: $3 H_2 + N_2 -$

Conversion factor:

Mole ratio between unknown substance (<mark>ammonia</mark>) and known substance (hydrogen): 2 moles NH₃

3 moles H₂

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8.00 moles H_2 $\begin{bmatrix} 2 \text{ moles } NH_3 \\ \hline 3 \text{ moles } H_2 \end{bmatrix} = 5.33 \text{ moles } NH_3$

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Remember the baking analogy?



How many eggs do you need to make 60 pancakes?

Conversion factor between eggs and pancakes:

6 eggs

24 pancakes





How many moles of silver nitrate $(AgNO_3)$ are required to produce 100.0 g of silver sulfide (Ag_2S) ?

$$2 \text{ AgNO}_3 + \text{H}_2\text{S} \longrightarrow \text{Ag}_2\text{S} + 2 \text{ HNO}_3$$

<u>Step 1:</u> Convert the amount of known substance (Ag_2S) from grams to moles



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<u>Step 2:</u> Determine the number of moles of the unknown substance $(AgNO_3)$ required to produce the number of moles of the known substance (0.403 mol Ag₂S)

Conversion Factor:





Mass - mass calculation: Another example

How many grams of carbon dioxide are produced by the complete combustion of 100. g of pentane (C_5H_{12}) ?

The balanced equation is:

 $C_5H_{12}(g) + 8O_2(g) \longrightarrow 5CO_2(g) + 6H_2O(g)$

Step 1: Convert the amount of known substance (C_5H_{12}) from grams to moles

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Molar mass C_5H_{12}: (5 x 12.01 g/mol) + (12 x 1.008 g/mol)
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= 72.15 g/mol

 $100. \underline{gC_{5}H_{12}} = \frac{1 \mod C_{5}H_{12}}{72.15 \underline{gC_{5}H_{12}}} = 1.39 \mod C_{5}H_{12}$

Mass - mass calculation: Another example

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The balanced equation is:

 $C_5H_{12}(g) + 8O_2(g) \longrightarrow 5CO_2(g) + 6H_2O(g)$

<u>Step 3:</u> Convert the amount of unknown substance (6.95 moles CO_2) from moles to grams

Molar mass CO₂: 12.01 g/mol + $(2 \times 16.00 \text{ g/mol}) = 44.01 \text{ g/mol}$



Mass - mass calculation: Another example

How many grams of carbon dioxide are produced by the complete combustion of 100. g of pentane (C_5H_{12}) ?

The balanced equation is:

$$C_5H_{12}(g) + 8 O_2(g) \longrightarrow 5 CO_2(g) + 6 H_2O(g)$$

Step 2: Determine the number of moles of the unknown substance (CO₂) required to produce the number of moles of the known substance $(1.39 \text{ mol } C_5H_{12})$

Conversion Factor:



Yields

Theoretical yield -- the calculated amount (mass) of product that can be obtained from a given amount of reactant based on the balanced chemical equation for a reaction

Actual yield -- the amount of product actually obtained from a reaction

The actual yield observed for a reaction is almost always less than the theoretical yield due to:

- side reactions that form other products
- incomplete / reversible reactions
- loss of material during handling and transfer from one vessel to another

The actual yield should never be greater than the theoretical yield

- if it is, it is an indicator of experimental error

Percent yield = 100 x ...

theoretical yield

Yields Yields Silver bromide was prepared by reacting 200.0 g of magnesium Silver bromide was prepared by reacting 200.0 g of magnesium bromide and an excess amount of silver nitrate. bromide and an excess amount of silver nitrate. Equation: MgBr₂ + 2 AgNO₃ \longrightarrow Mg(NO₃)₃ + 2 AgBr Equation: MgBr₂ + 2 AgNO₃ \longrightarrow Mg(NO₃)₃ + 2 AgBr a) What is the theoretical yield of silver bromide? a) What is the theoretical yield of silver bromide? Step 2: Determine how many moles of AgBr can be formed from Step 1: Convert the amount of MgBr₂ from grams to moles this amount of MgBr₂ (i.e., 1.086 moles) $1.086 \text{ mol-MgBr}_2 \left[\frac{2 \text{ mol AgBr}}{1 \text{ mol-MgBr}_2} \right] = 2.172 \text{ mol AgBr}$ $200.0 g MgBr_{2}$ (1 mol MgBr_{2} / 184.1 g MgBr_{2}) = 1.086 mol MgBr_{2} This is the theoretical yield Step 3: Convert from moles to grams = 407.9 g AgBr 2.172 mol AgBr (187.8 g AgBr / 1 mol AgBr) 21 22 The concept of limiting reactants **Yields** Silver bromide was prepared by reacting 200.0 g of magnesium In some chemical reactions, all reagents are present in the exact bromide and an excess amount of silver nitrate. amounts required to completely react with one another. Equation: MgBr₂ + 2 AgNO₃ \longrightarrow Mg(NO₃)₃ + 2 AgBr

Example: In a lab experiment, ammonia is produced by reacting 6.05 g of hydrogen gas (3 moles) with 28.02 g of nitrogen gas (1 mole)

 $3 H_2 + N_2 \longrightarrow 2 NH_3$

In this case, hydrogen and nitrogen are said to react in stoichiometric amounts

b) Calculate the percent yield if 375.0 g of silver bromide was

actual vield percent yield = 100 x

theoretical vield

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percent yield = $100 \times$

obtained from the reaction

The concept of *limiting reactants*

But in many cases, a chemical reaction will take place under conditions where one (or more) of the reactants is present *in excess*

-- *i.e.*, there is more than enough of that reactant available for the reaction to proceed

Example: Combustion of 85.0 g of propane in air

$$C_3H_8(g) + 5 O_2(g) \longrightarrow 3 CO_2(g) + 4 H_2O(g)$$

There is more than enough oxygen available in the air to react with all of the propane

-- the reaction will proceed until all of the 85.0 g of propane has been consumed

Another food analogy...

Recipe for a grilled cheese sandwich:

Two slices bread and one slice of cheese gives one sandwich

Balanced equation:



If you have 10 slices of bread and 4 slices of cheese, how many sandwiches can you make?

- enough bread for (10 / 2) = 5 sandwiches
- enough cheese for (4/1) = 4 sandwiches
- · you can only make 4 sandwiches before the cheese is used up
- · cheese is the limiting reactant

The concept of *limiting reactants*

But in many cases, a chemical reaction will take place under conditions where one (or more) of the reactants is present in excess

-- *i.e.,* there is more than enough of that reactant available for the reaction to proceed

The limiting reactant is the reactant that is <u>not</u> present in excess

- -- the limiting reactant will be used up first (the reaction will stop when the limiting reactant is depleted)
- -- the limiting reactant therefore limits the amount of product that can be formed by the reaction

In the previous example, **propane** was the **limiting reactant** (oxygen was present in excess)

$$C_3H_8(g)$$
 + 5 $O_2(g)$ \longrightarrow 3 $CO_2(g)$ + 4 $H_2O(g)$

Another food analogy...

Recipe for a grilled cheese sandwich:

Two slices bread and one slice of cheese gives one sandwich

Balanced equation:



If you have 8 slices of bread and 6 slices of cheese, how many sandwiches can you make?

- enough bread for (8 / 2) = 4 sandwiches
- enough cheese for (6 / 1) = 6 sandwiches
- · you can only make 4 sandwiches before the bread is used up
- bread is the limiting reactant

Limiting reactants

Chemistry example:

Hydrogen and chlorine gas combine to form hydrogen chloride:

 $H_2 + Cl_2 \longrightarrow 2 HCl$

If 4 moles of hydrogen reacts with 3 moles of chlorine, how many moles of HCl will be formed?



Limiting reactants

Chemistry example:

Hydrogen and chlorine gas combine to form hydrogen chloride:

 $H_2 + Cl_2 \longrightarrow 2 HCl$

If 4 moles of hydrogen reacts with 3 moles of chlorine, how many moles of HCl will be formed?

8 mol HCl can be formed from 4 mol of $\rm H_2$

6 mol HCl can be formed from 3 mol of $\rm Cl_2$

3 moles of H_2 will react with 3 moles of Cl_2

- At this point, the Cl₂ will have been completely consumed and the reaction stops (chlorine is the *limiting reactant*)
- 1 mole of H₂ will remain unreacted (hydrogen is present in excess)
- 6 moles of HCI will have been formed

Procedure for identifying the limiting reactant

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- 1. Calculate the amounts of *product* that can be formed from each of the reactants
- 2. Determine which reactant gives the <u>least amount of</u> product -- this is the limiting reactant

Do <u>not</u> just compare the numbers of moles of reactants -- you must also account for the ratios in which the reactants combine

- 3. To find the amount of the non-limiting reactant remaining after the reaction:
 - -- calculate the amount of the non-limiting reactant required to react completely with the limiting reactant
 - -- subtract this amount from the starting quantity of the non-limiting reactant



Limiting reactant

How many grams of silver bromide (AgBr) can be formed when solutions containing 55.0 g of $MgBr_2$ and 95.0 g of $AgNO_3$ are mixed together?

<u>Equation:</u> MgBr₂ + 2 AgNO₃ \longrightarrow 2 AgBr + Mg(NO₃)₂

How many grams of the excess reactant remain unreacted?

Since $AgNO_3$ is the limiting reactant, all 95.0 g of $AgNO_3$ will be used up. Calculate how much $MgBr_2$ (the excess reactant) is required to react with 95.0 g $AgNO_3$ and then determine how much $MgBr_2$ is left over.

Remember that in the previous steps, we calculated that $95.0 \text{ g of } AgNO_3$ is equal to 0.559 moles of $AgNO_3$.

So we first need to determine how many moles of $MgBr_2$ are required to react with 0.559 moles of $AgNO_3$

-- then convert to grams and subtract from the original amount of MgBr2

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Gravimetric analysis

Gravimetric analysis is a chemical analytical method based on the measurement of <u>masses</u>

• it can be used in combination with precipitation reactions to determine the amount of dissolved substances present in a solution



Limiting reactant

How many grams of silver bromide (AgBr) can be formed when solutions containing 55.0 g of $MgBr_2$ and 95.0 g of $AgNO_3$ are mixed together?

<u>Equation:</u> $MgBr_2 + 2 AgNO_3 \longrightarrow 2 AgBr + Mg(NO_3)_2$

How many grams of the excess reactant remain unreacted?

 $0.559 \text{ mol AgNO}_{3} \left[\frac{1 \text{ mol MgBr}_{2}}{2 \text{ mol AgNO}_{3}} \right] = 0.280 \text{ mol MgBr}_{2}$

 0.280 mol MgBr_2 (184.11 g MgBr₂ / 1 mol MgBr₂) = 51.5 g MgBr₂

When all 95.0 g of $AgNO_3$ has reacted, 51.5 g of $MgBr_2$ will have been consumed. The amount of unreacted $MgBr_2$ left over is given by:

 $55.0 \text{ g} - 51.5 \text{ g} = 3.5 \text{ g} \text{ MgBr}_2$

Example: A 1-liter sample of industrial wastewater is analyzed for lead (in its Pb²⁺ ionic form) by gravimetric analysis.

This is done by adding excess sodium sulfate to the water sample to precipitate lead (II) sulfate.

The mass of PbSO₄ produced is 300.0 mg. **Calculate the** mass of lead in the water sample.

<u>Solution</u>: The dissolved Pb^{2+} ions in the water sample will react with the SO_4^{2-} ions added as sodium sulfate to form insoluble $PbSO_4$

<u>Net ionic equation</u>: $Pb^{2+}(aq) + SO_4^{2-}(aq) \longrightarrow PbSO_4(s)$

This is a mass-mass stoichiometry problem

It also involves a limiting reactant, but the problem statement tells you what it is beforehand - i.e., $Pb^{2+}(aq)$

