Chem 103, Section F0F
Unit IV - Stoichiometry of Formulas and Equations
Lecture 12

- Writing and balancing chemical equations
- Calculating the amounts of reactant consumed and products formed in a chemical reaction
- Carrying out reactions in solution

Lecture 12 - Stoichiometry

Reading in Silberberg

- Chapter 3, Section 3
  - Writing and Balancing Chemical Equations
- Chapter 3, Section 4
  - Calculating Amounts of Reactant and Product
- Chapter 3, Section 5
  - Fundamentals of Solution Stoichiometry

Lecture 12 - Introduction

Stoichiometry is the study of the quantitative aspects of chemical formulas and chemical reactions.

- Using the tools of stoichiometry, you can predict the quantities of reactants and products that can be consumed or produced in a chemical reaction.
- These calculations will require working with *chemical formulas* and *balanced chemical reactions*.

Lecture 12 - Writing and Balancing Chemical Equations

While mass is conserved in a chemical reaction

- so is the number and types of atoms that participate in a chemical reaction.

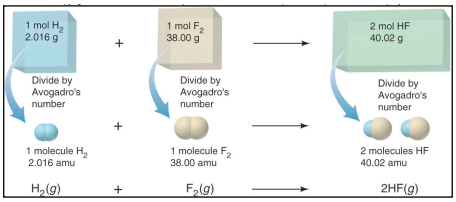
From Dalton's postulates:

- In a chemical process, atoms cannot be created, destroyed, or change, only rearranged into different combinations.
- A molecular formula (covalent compounds) or a formula unit (ionic compounds) represents a fixed ratio of the elements in a compound, so a different ratio represents a different compound.

Lecture 12 - Writing and Balancing Chemical Equations

Focusing on the numbers instead of masses provides more information about a reaction.

- This is embodied in the **balanced chemical equation** for a reaction
  - An equation is balanced when all of the atoms on the reactant side of the equation are found on the product side of the equation.



Lecture 12 - Writing and Balancing Chemical Equations

Balanced chemical equations have many of the properties of arithmetic equations.

- For example, they can be added together to get the net reaction equation for a series of reactions

$$\begin{array}{rcl} A + B & = & \not{\varnothing} + D \\ \not{\varnothing} + E & = & F + G \\ \hline A + B + E & = & D + F + G \end{array}$$

Lecture 12 - Writing and Balancing Chemical Equations

Demonstration
- The oxidation of Magnesium

Reaction statement
- Solid Magnesium metal (Mg) reacts with oxygen gas (O_2) to produce solid magnesium oxide (MgO)

Lecture 12 - Writing and Balancing Chemical Equations

Steps to writing a balanced chemical equation:
1. Translate the chemical statement into a skeleton equation.

$$Mg + O_2 \longrightarrow MgO$$

Lecture 12 - Writing and Balancing Chemical Equations

Steps to writing a balanced chemical equation:
2. Balance the atoms by adding coefficients
   - Start with the most complicated substance (MgO) and work to the simpler ones:

$$Mg + O_2 \longrightarrow MgO$$
$$Mg + O_2 \longrightarrow 1\ MgO$$
$$1\ Mg + O_2 \longrightarrow 1\ MgO$$
$$1\ Mg + 1/2\ O_2 \longrightarrow 1\ MgO$$

Lecture 12 - Writing and Balancing Chemical Equations

Steps to writing a balanced chemical equation:
3. Adjust the coefficients to get the smallest set of integer coefficients.
   - Do this by multiplying all the coefficients by the same integer.

$$1\ Mg + 1/2\ O_2 \longrightarrow 1\ MgO$$
$$2\ Mg + 1\ O_2 \longrightarrow 2\ MgO$$
$$2\ Mg + O_2 \longrightarrow 2\ MgO$$

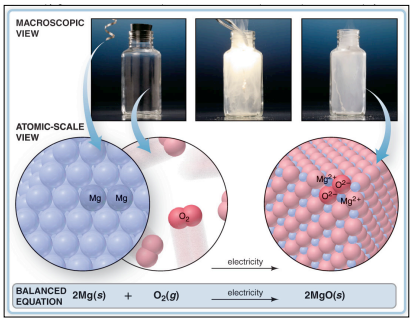
Lecture 12 - Writing and Balancing Chemical Equations

Steps to writing a balanced chemical equation:
4. Finish off by indicating the state of each reactant and product.
   - solid (*s*)
   - gas (*g*)
   - liquid (*l*)

$$2\ Mg(s) + O_2(g) \longrightarrow 2\ MgO(s)$$

Lecture 12 - Writing and Balancing Chemical Equations

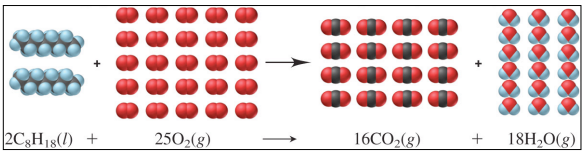
Balanced chemical equations give us insight into what is happening at the molecular level.



Lecture 12 - Writing and Balancing Chemical Equations

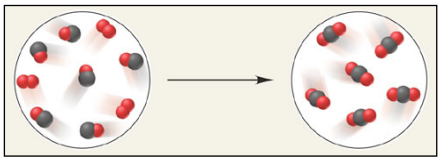
Balanced chemical equations give us insight into what is happening at the molecular level.

- Combustion of octane (C_8H_{18}), a component of a gasoline



Lecture 12 - Question 1

Write a balanced equation for the important atmospheric reaction depicted below (carbon is black; oxygen is red)



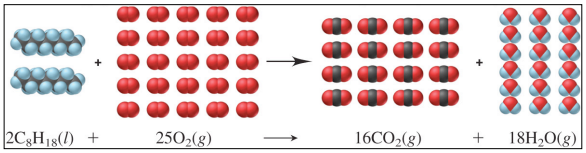
Lecture 12 - Calculating Amounts of Reactant and Product

Stoichiometrically Equivalent Amounts

- *A definite amount of one substance that is formed from, produces, or reacts with a definite amount of an another substance, in a chemical reaction*.
- The stoichiometrically equivalent amounts are given by the coefficients in a balanced chemical equations.

Lecture 12 - Calculating Amounts of Reactant and Product

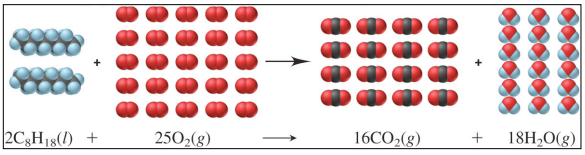
- For example, with the combustion of octane:



- 2 mol of C_8H_{18} reacts with 25 mol of O_2.
- 2 mol of C_8H_{18} produces 16 mol of CO_2.
- 2 mol of C_8H_{18} produces 18 mol of H_2O.

Lecture 12 - Calculating Amounts of Reactant and Product

- Another way to express this is

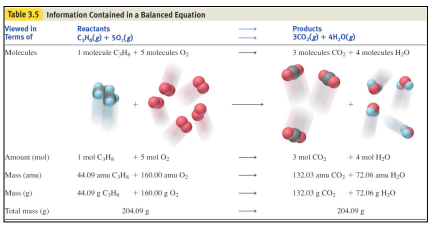


- 2 mol of C_8H_{18} is *stoichiometrically equivalent to* 25 mol of O_2.
- 2 mol of C_8H_{18} is *stoichiometrically equivalent to* 16 mol of CO_2.
- 2 mol of C_8H_{18} is *stoichiometrically equivalent to* 18 mol of H_2O.

Lecture 12 - Calculating Amounts of Reactant and Product

The information contained in the balanced chemical reaction:

- For example, the combustion of propane (C_3H_8):



- The stoichiometric equivalents can be used to create conversion factors for solving stoichiometry problems.

Lecture 12 - Question 2

In the combustion of propane (C_3H_8), how many moles of O_2 are consumed when 10.0 mol of H_2O are produced.

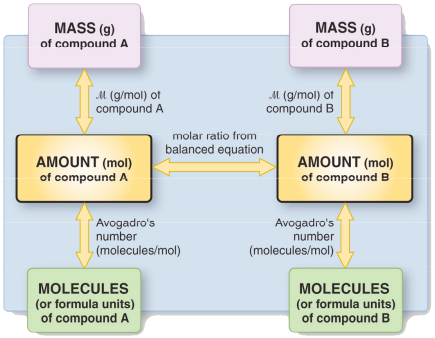
Lecture 12 - Calculating Amounts of Reactant and Product

The general steps that should be followed for these types of problems is

1. Write a balanced equation for the reaction.
2. Convert the given mass (or number of entities) of the first substance to an amount (mol).
3. Use the appropriate molar ratio from the balanced equation to calculate the amount (mol) of the second substance.
4. Convert the amount of the second substance to the desired mass (or number of entities).

Lecture 12 - Calculating Amounts of Reactant and Product

This process is represented in the following flowchart:



Lecture 12 - Clicker Question 3

Thermite is a mixture of iron(III) oxide and aluminum powders that was once used to weld railroad tracks. It undergoes a spectacular reaction to yield solid aluminum oxide and molten iron.

- What is ratio of the number of moles of iron formed from each mole of aluminum consumed in this reaction?

A) $\left(\frac{2\text{ mol Fe}}{1\text{ mol Al}}\right)$

B) $\left(\frac{1\text{ mol Fe}}{1\text{ mol Al}}\right)$

C) $\left(\frac{1\text{ mol Fe}}{3\text{ mol Al}}\right)$

D) $\left(\frac{3\text{ mol Fe}}{1\text{ mol Al}}\right)$

Lecture 12 - Question 3

Thermite is a mixture of iron(III) oxide and aluminum powders that was once used to weld railroad tracks. It undergoes a spectacular reaction to yield solid aluminum oxide and molten iron.

- How many grams of iron form when 135 g of aluminum reacts?

Lecture 12 - Calculating Amounts of Reactant and Product

Many reactions occur in sequences.

- This is particularly the case in biochemistry.
- Such sequence of reactions are called **pathways**.

The chemical equations can be added together to get an overall or net equation for the pathway.

- For this to work, at least one of the products for a reaction in the pathway must be a reactant in the subsequent reaction.

Lecture 12 - Question 4

Metallic copper can be extracted from copper(I) sulfide ores by reacting the copper(I) sulfide with oxygen. One of the products of this reaction is sulfur dioxide (SO_2):

$$2\,Cu_2S + 3\,O_2 + 2\,C \longrightarrow 2\,SO_2 + 4\,Cu + 2\,CO$$

The SO_2 produced can then react with oxygen to produce sulfur trioxide (SO_3).

If the sulfur trioxide (SO_3), which is a gas, is released into the air, it can then react with water vapor to produce sulfuric acid (H_2SO_4). This is a major contributor to acid rain

- Write the net reaction equation for this sequence of reactions

Lecture 12 - Calculating Amounts of Reactant and Product

In metabolism, the oxidation of glucose ($C_6H_{10}O_6$) to CO_2 and H_2O is a major source of chemical energy for living organisms.

- The net reaction equation for this reaction is

$$C_6H_{12}C_6 + 6\,O_2 \longrightarrow 6\,CO_2 + 6\,O_2$$

Lecture 12 - Calculating Amounts of Reactant and Product

In order for this energy to be extracted in a usable form, the oxidation of glucose is broken down into many steps:

1. Glycolysis (10 reactions)

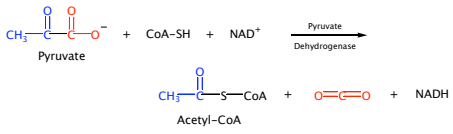
TABLE 16.3 Reactions of glycolysis

Step	Reaction	Enzyme	Reaction type	$\Delta G'^{\circ}$ in kcal mol^{-1} (kJ mol^{-1})	ΔG in kcal mol^{-1} (kJ mol^{-1})
1	Glucose + ATP ⟶ glucose 6-phosphate + ADP + H^+	Hexokinase	Phosphoryl transfer	−4.0 (−16.7)	−8.0 (−33.5)
2	Glucose 6-phosphate ⟺ fructose 6-phosphate	Phosphoglucose isomerase	Isomerization	+0.4 (+1.7)	−0.6 (−2.5)
3	Fructose 6-phosphate + ATP ⟶ fructose 1,6-bisphosphate + ADP + H^+	Phosphofructokinase	Phosphoryl transfer	−3.4 (−14.2)	−5.3 (−22.2)
4	Fructose 1,6-bisphosphate ⟺ dihydroxyacetonephosphate + glyceraldehyde 3-phosphate	Aldolase	Aldol cleavage	+5.7 (+23.8)	−0.3 (−1.3)
5	Dihydroxyacetone phosphate ⟺ glyceraldehyde 3-phosphate	Triose phosphate isomerase	Isomerization	+1.8 (+7.5)	+0.6 (+2.5)
6	Glyceraldehyde 3-phosphate + P_i + NAD^+ ⟺ 1,3-bisphosphoglycerate + NADH + H^+	Glyceraldehyde 3-phosphate dehydrogenase	Phosphorylation coupled to oxidation	+1.5 (+6.3)	+0.6 (+2.5)
7	1,3-Bisphosphoglycerate + ADP ⟺ 3-phosphoglycerate + ATP	Phosphoglycerate kinase	Phosphoryl transfer	−4.5 (−18.8)	+0.3 (+1.3)
8	3-Phosphoglycerate ⟺ 2-phosphoglycerate	Phosphoglycerate mutase	Phosphoryl shift	+1.1 (+4.6)	+0.2 (+0.8)
9	2-Phosphoglycerate ⟺ phosphoenolpyruvate + H_2O	Enolase	Dehydration	+0.4 (+1.7)	−0.8 (−3.3)
10	Phosphoenolpyruvate + ADP + H^+ ⟶ pyruvate + ATP	Pyruvate kinase	Phosphoryl transfer	−7.5 (−31.4)	−4.0 (−16.7)

Lecture 12 - Calculating Amounts of Reactant and Product

In order for this energy to be extracted in a usable form, the oxidation of glucose is broken down into many steps:

2. Conversion of pyruvate to acetyl-CoA (1 reaction)



Lecture 12 - Calculating Amounts of Reactant and Product

In order for this energy to be extracted in a usable form, the oxidation of glucose is broken down into many steps:

3. Citric acid cycle (8 reactions)

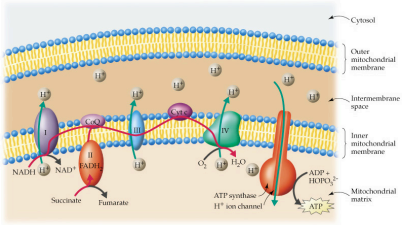
TABLE 17.2 Citric acid cycle

Step	Reaction	Enzyme	Prosthetic group	Type*	$\Delta G'^{\circ}$ kcal mol^{-1}	$\Delta G'^{\circ}$ kJ mol^{-1}
1	Acetyl CoA + oxaloacetate + H_2O ⟶ citrate + CoA + H^+	Citrate synthase		a	−7.5	−31.4
2a	Citrate ⟺ *cis*-aconitate + H_2O	Aconitase	Fe–S	b	+2.0	+8.4
2b	*cis*-Aconitate + H_2O ⟺ isocitrate	Aconitase	Fe–S	c	−0.5	−2.1
3	Isocitrate + NAD^+ ⟺ α-ketoglutarate + CO_2 + NADH	Isocitrate dehydrogenase		d + e	−2.0	−8.4
4	α-Ketoglutarate + NAD^+ + CoA ⟺ succinyl CoA + CO_2 + NADH	α-Ketoglutarate dehydrogenase complex	Lipoic acid, FAD, TPP	d + e	−7.2	−30.1
5	Succinyl CoA + P_i + GDP ⟺ succinate + GTP + CoA	Succinyl CoA synthetase		f	−0.8	−3.3
6	Succinate + FAD (enzyme-bound) ⟺ fumarate + $FADH_2$ (enzyme-bound)	Succinate dehydrogenase	FAD, Fe–S	e	−0	0
7	Fumarate + H_2O ⟺ L-malate	Fumarase		c	−0.9	−3.8
8	L-Malate + NAD^+ ⟺ oxaloacetate + NADH + H^+	Malate dehydrogenase		e	+7.1	+29.7

Lecture 12 - Calculating Amounts of Reactant and Product

In order for this energy to be extracted in a usable form, the oxidation of glucose is broken down into many steps:

4. Oxidative Phosphorylation (6 electron carriers)



Lecture 12 - Calculating Amounts of Reactant and Product

The **limiting reagent**

- The limiting reagent is the the reactant that will be used up first in a reaction.
  - It will determine how much product is produced.
  - Among all of the reactants, it is the one that will yield the lowest amount of product.

Lecture 12 - Clicker Question 5

Chlorine trifluoride (ClF_3) is used in processing uranium and is produced by reacting chlorine gas (Cl_2) with fluorine gas (F_2)

When the reaction is run with 0.750 mol of Cl_2 and 3.00 mol of F_2, what mass of chlorine trifluoride will be prepared?

Step 1: Which reactant is the limiting reactant?

A) Cl_2

B) F_2

C) Neither, they are stoichiometrically equivalent.

Lecture 12 - Calculating Amounts of Reactant and Product

The **theoretical yield**

- The amount of product produced when all of the limiting reagent is used up and converted to the desired product.
  - This is the maximum possible yield.
  - The actual yield is equal to or less than the theoretical yield, usually less than.

The **percent yield** is used to compare the actual yield to the theoretical yield:

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

Lecture 12 - Clicker Question 6

Marble (calcium carbonate) reacts with a hydrochloric acid solution to form a calcium chloride solution, water and carbon dioxide.

What is the percent yield of carbon dioxide if 3.65 g of gas is collected when 10.0 g of marble reacts.

A) 100%

B) 120%

C) 83%

D) 0%

Lecture 12 - Fundamentals of Solution Stoichiometry

Much of the chemistry that takes place in the lab is carried out in solution.

- It is much more convenient to measure the concentrations of reactants accurately using solutions.
- A solution is a mixture in which the components of the mixture are dispersed homogeneously at the molecular level.
  - The component that is present in the larger amount is called the **solvent**.
  - The component that is present in smaller quantities is called the **solute**.
- The solvent often does not participate directly in solution reactions.

Lecture 12 - Fundamentals of Solution Stoichiometry

The concentration of solution expresses the amount of solute dissolved in a given amount of solution.

- We most often use **molarity**, which is defined as

$$\text{Molarity} = \frac{\text{moles of solute}}{\text{liters of solution}}$$

Lecture 12 - Clicker Question 7

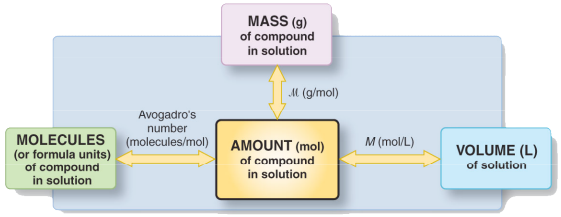
Glycine (H_2NCH_2COOH) is the simplest amino acid.

What is the molarity of an aqueous solution that contains 0.715 mol of glycine in 495 mL?

A) 0.715 M
B) 2.0 M
C) 1.44 M
D) 495 M

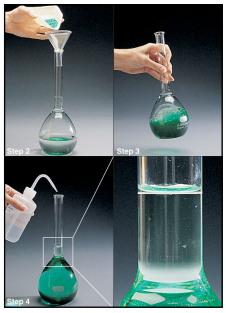
Lecture 12 - Fundamentals of Solution Stoichiometry

Molarity can be thought of as another conversion factor in stoichiometry problems.



Lecture 12 - Question 8

What mass of citric acid (C6H8O7) is needed to make up 25.0 mL of a 1.0 M solution of citric acid in water.



Lecture 12 - Fundamentals of Solution Stoichiometry

When diluting a solution, solvent is added to increase the volume of the solution

- The number of solute molecules remains the same:

$$M_{conc} \times V_{conc} = \text{moles of solute} = M_{dilute} \times V_{dilute}$$

Lecture 12 - Question 9

What is the volume of 2.050 M copper(II) nitrate that must be diluted with water to prepare 750.0 mL of a 0.8543 M solution of copper(II) nitrate?

Lecture 12 - Fundamentals of Solution Stoichiometry

Reactions in Solution

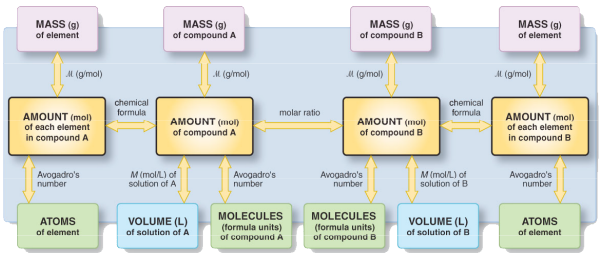
- You may need to convert volumes to moles and *vice versa*.
  - The concentrations are used as the conversion factors in these calculations.

Lecture 12 - Question 10

How many grams of NaH_2PO_4 are needed to react with 43.74 mL of 0.285 M NaOH.

Lecture 12 - Fundamentals of Solution Stoichiometry

To Summarize:



Unit IV - Up Next

Unit V - Chemical Reactions and Chemical Properties

- Mixtures
- Water as the solvent in a solution mixture
- Reactions of ionic compounds in solution
- Reactions of acids and Bases

The End