

We can calculate the MASS FRACTION of each component, then multiply the mass fraction by 56 g (the sample's actual mass) to get the mass of each component.

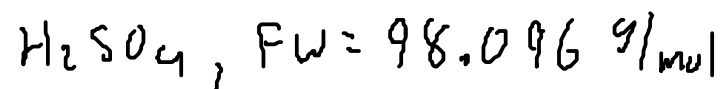
$$\text{mass fraction } C_3H_8 = \frac{22.48794 \text{ g } C_3H_8}{50.96674 \text{ g total}} = 0.4412277497$$

$$\text{mass } C_3H_8 = 56 \text{ g} \times 0.4412277497 = 24.71 \text{ g } C_3H_8$$

$$\text{mass } C_4H_{10} = 56 \text{ g} - 24.71 \text{ g} = 31.29 \text{ g } C_4H_{10}$$

So, 25 g C_3H_8 + 31 g C_4H_{10}

Commercial sulfuric acid (98% by mass) is 18 M. What is the density of the solution, and what is the molality?



$$\text{want: density} = \frac{\text{mass solution}}{\text{volume solution}}$$

Let's start with MOLARITY ... since it's the only thing we know about the solution that relates to volume. Assume a basis of 1L solution...

$$\text{know } 18 \text{ M} = \frac{\text{mol H}_2\text{SO}_4}{\text{L solution}}$$

$$98\% = \frac{\text{g H}_2\text{SO}_4}{100 \text{ g solution}}$$

$$1 \text{ L} \times \frac{18 \text{ mol H}_2\text{SO}_4}{\text{L}} = 18 \text{ mol H}_2\text{SO}_4$$

We can find the mass sulfuric acid from the moles, then take advantage of the fact that it's a 98% solution!

$$18 \text{ mol H}_2\text{SO}_4 \times \frac{98.096 \text{ g H}_2\text{SO}_4}{\text{mol H}_2\text{SO}_4} = 1765.728 \text{ g H}_2\text{SO}_4$$

Since the solution is 98% sulfuric acid ...

$$0.98 = \frac{1765.728 \text{ g H}_2\text{SO}_4}{\text{mass solution}}; \text{ mass solution} = 1801.763265 \text{ g solution}$$

$$\text{density} = \frac{\text{mass solution}}{\text{volume solution}} = \frac{1801.763265 \text{ g solution}}{1000 \text{ mL}} = \boxed{1.8 \text{ g/mL}}$$

$$\text{molality} = \frac{\text{mol H}_2\text{SO}_4}{\text{kg H}_2\text{O}}$$

If we keep our original basis of 1L solution, we already know the moles sulfuric acid and the masses of both the sulfuric acid and the solution.

So, we can find the mass of water by subtraction

$$\begin{aligned} 1801.763265 \text{ g solution} - 1765.728 \text{ g H}_2\text{SO}_4 &= \\ = 36.03526531 \text{ g H}_2\text{O} &= 0.03603526531 \text{ kg H}_2\text{O} \end{aligned}$$

So, molality is ...

$$\frac{18 \text{ mol H}_2\text{SO}_4}{0.03603526531 \text{ kg H}_2\text{O}} = \boxed{500 \text{ m H}_2\text{SO}_4}$$

KINETICS

- the study of the RATE of chemical reactions. Or, the study of the factors affecting how fast chemical reactions proceed.

DEFINING RATE

- RATE is defined as the change in the molar (M) concentration of a reactant or product over time. Usually, rate is defined in terms of one of the REACTANTS



...Let's look at a simple combination

$$\text{Rate} = \frac{-\Delta[A]}{\Delta t}$$

$[A]$ = "molar concentration of substance "A".

Square brackets () are used to denote MOLAR concentration

change in time

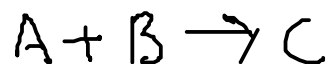
$$\text{Rate} = \frac{\Delta[C]}{\Delta t}$$

You could ALSO define the rate in terms of the disappearance of B or the appearance of C over time! Our choice of A was arbitrary,

Negative sign because we define the rate as a POSITIVE number, and (A) will decrease over time!

THE RATE LAW

- We express the rate of reaction using an equation called the RATE LAW.



$$\text{Rate} = - \frac{\Delta[A]}{\Delta t} = k \times [A]^p \times [B]^q$$

This is the RATE CONSTANT. It depends on TEMPERATURE, but does not depend on the CONCENTRATION of any reactant or product.

"p" and "q" are called REACTION ORDERS. They indicate the effect a particular reactant or catalyst has on the rate of a reaction. Reaction orders may be positive, zero (in which case the substance has NO effect on rate) and negative (in which case the substance actually slows the reaction down).

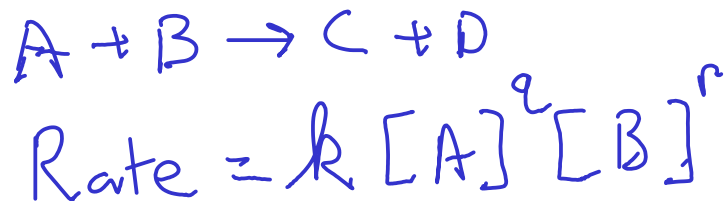
- Rate laws depend on CONCENTRATION of reactants. Since the concentrations of reactants CHANGE throughout the course of the reaction, so does the rate!
- RATE CONSTANTS and REACTION ORDERS are determined experimentally. If you do experiment 13 (the iodine clock reaction), you will see how this can be done in the lab via the INITIAL RATES METHOD.

Initial rates method:

- To determine the rate constant and reaction orders in a reaction, it's possible to monitor the rate of a reaction starting from time zero to a short time later where the concentrations of the reactants haven't changed much. In other words, we look at the INITIAL RATE.

- To determine the rate constant and orders, we need to perform several experiments - one for each order to determine and one baseline experiment to determine the rate constant.

Example:



... we want to find the rate constant 'k', and the orders 'q' and 'r'.

Trial	[A]	[B]	Rate $-\frac{\Delta [A]}{s}$
1	0.150	0.150	Baseline experiment
2	0.300	0.150	Double (A) to find 'q'
3	0.150	0.300	Double (B) to find 'r'

Trial	[A]	[B]	Rate $-\frac{\Delta [A]}{s}$
1	0.150	0.150	0.0016875
2	0.300	0.150	0.0033750
3	0.150	0.300	0.0067500

Rate doubles (from trial 1 to 2)
Rate quadruples (from trial 1 to 3)

The rate law is:

$$\text{Rate} = k [A]^q [B]^r$$

... so how do we use the data above to find out the values of 'k', 'q', and 'r'?

We observe that in the second trial ((A) doubled), the rate has doubled!

$$(2 \times [A])^q = 2 \times \text{Rate} ; q = 1$$

We observe that in the third trial ((B) doubled), the rate has quadrupled.

$$(2 \times [B])^r = 4 \times \text{Rate} ; r = 2$$

$$\text{Rate} = k [A] [B]^2$$

Trial	[A]	[B]	Rate $\frac{\Delta [A]}{s}$	Calculated 'k'
1	0.150	0.150	0.0016875	0.500
2	0.300	0.150	0.0033750	0.500
3	0.150	0.300	0.0067500	0.500

$$\text{Rate} = k [A][B]^2$$

Now, we'd like to know the value of 'k'. Solve rate law for 'k'.

$$k = \frac{\text{Rate}}{[A][B]^2}$$

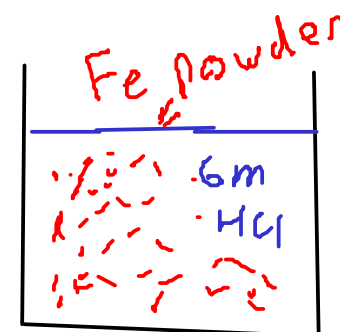
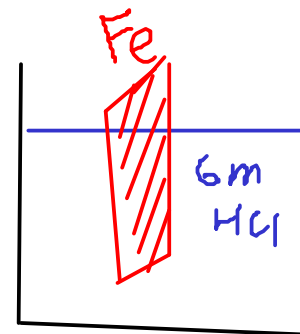
Plug in each set of data to this equation and calculate 'k'!

The average of these calculated 'k' values equals the rate constant.
(For real data, expect some experimental error in these numbers!)

$$\text{Rate} = 0.500 [A][B]^2$$

FACTORS THAT AFFECT REACTION RATE

- ① CONCENTRATION OF REACTANTS
- ② SURFACE AREA OF CONTACT BETWEEN REACTANTS
- ③ CONCENTRATION OF / PRESENCE OF A CATALYST
- ④ TEMPERATURE



CONCENTRATION OF REACTANTS

- Usually, the reaction rate increases as you increase the concentration of a reactant. This is true if the order for that reactant is greater than zero!

$$\text{Rate} = k[A]^n$$

$$[A]^0$$

$$[A]^1$$

$$[A]^{-1} \quad \frac{1}{[A]}$$

If the order is 0 the value of this term will be 1 no matter what (A) is!

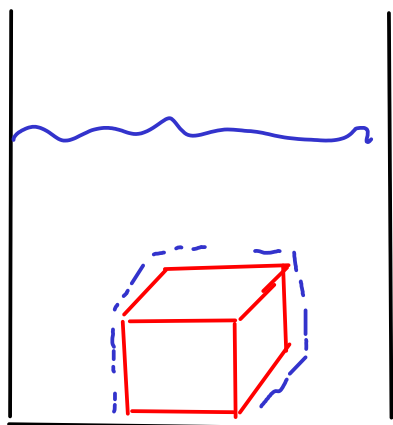
If the order is -1, this term will get SMALLER (reducing rate) as (A) gets larger!
"inhibitor"

- In most cases, reaction orders ARE positive numbers!

SURFACE AREA OF CONTACT BETWEEN REACTANTS

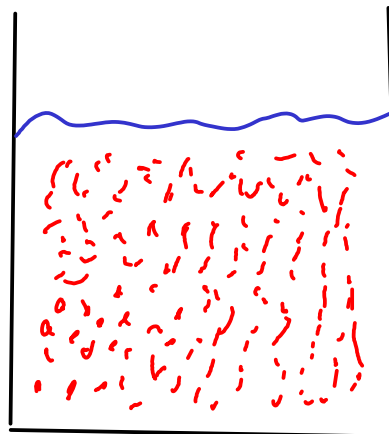
- If a reaction takes place at an INTERFACE, then the reaction rate will depend on the SURFACE AREA of that interface!

Consider a reaction between a liquid and a solid. The reaction can only take place where the liquid and the solid TOUCH each other,



The reaction takes place only on the surface of the cube.

Next, try the same reaction, but break the cube into small fragments first!



Here, the reaction takes place on the surface area of each fragment. In total, this is a much LARGER surface than the cube.

- The larger the SURFACE AREA of the INTERFACE between the reactants, the faster the reaction will occur!

- This is not an important factor for reactions that take place IN SOLUTION, since there is no interface.

CONCENTRATION OF / PRESENCE OF A CATALYST

- a CATALYST is a substance that INCREASES the rate of a reaction without being consumed in the reaction.

- Appear in the rate law equation, but are written as "reaction conditions" in traditional chemical equations. Typically, the higher the concentration of catalyst, the faster the reaction.



$$\text{Rate} = k [A]^p [B]^q [C]^r$$

└ The catalyst shows up in the rate law like the reactants!

- Work via many different mechanisms. Some provide surfaces for reactants to bind to and react. Some react with reactant molecules to leave them in a state more suitable for the main reaction (and are then regenerated during the main reaction). Some catalysts bind to and bend reactants into favorable orientations for reactions, etc.

- Biological catalysts are usually called ENZYMES.

TEMPERATURE

- We observe that chemical reactions proceed FASTER at HIGHER temperatures.

... but sometimes reactions are run at low temperatures for other reasons - like safety, decomposition of desired products at high temperatures, formation of competing undesirable products at high temperatures, etc.

Note: Changing temperature affects the RATE CONSTANT, k !

REACTION RATE THEORY

- We'd like to have an explanation for how the four factors we discussed affect the reaction rate!
- COLLISION THEORY and TRANSITION STATE THEORY attempt to explain reaction rate.

COLLISION THEORY

- states that for a reaction to occur between atoms or molecules, three things must occur:

- ① Reactants must COLLIDE with each other.
- ② Colliding reactants must hit each other with the correct ORIENTATION to react.
- ③ Colliding reactants must also hit each other with ENOUGH ENERGY to react (called the ACTIVATION ENERGY)