Chemical Kinetics

Topic 6.1 Collision theory and rates of reactions

Studying chemical reactions

- One of the questions that scientist have about a chemical reaction is ‘Does the reaction happen quickly or slowly?’
- Some reactions happen very quickly such as an air bag being inflated and some happen very slowly like the radioactive decay of carbon used in carbon dating.

Rate of reaction

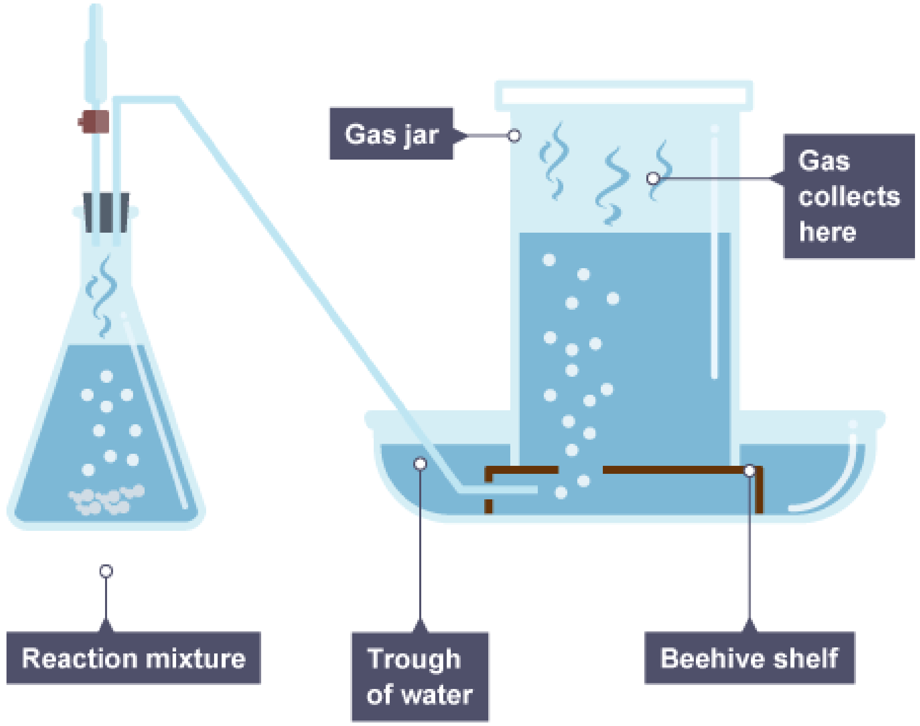
- Rate of reaction is defined as the change in concentration of reactants or products per unit time.
- The units are mol dm^{-1} s^{-1} or mol dm^{-1} min^{-1} etc.
- Change in concentration can be measured in a number of ways depending on the type of reactions
  - pH(acid-base)
  - Color change (transition metals)
  - Change in mass or volume(gas or solid)
  - Change in conductivity (electrolytes)

Determining rates of reaction

- Rate of reaction is usually determined using a graph where you measure the concentration change directly over time or one of the previously mentioned properties.
- The rate of reaction is the slope or the gradient of the tangential line at time T.

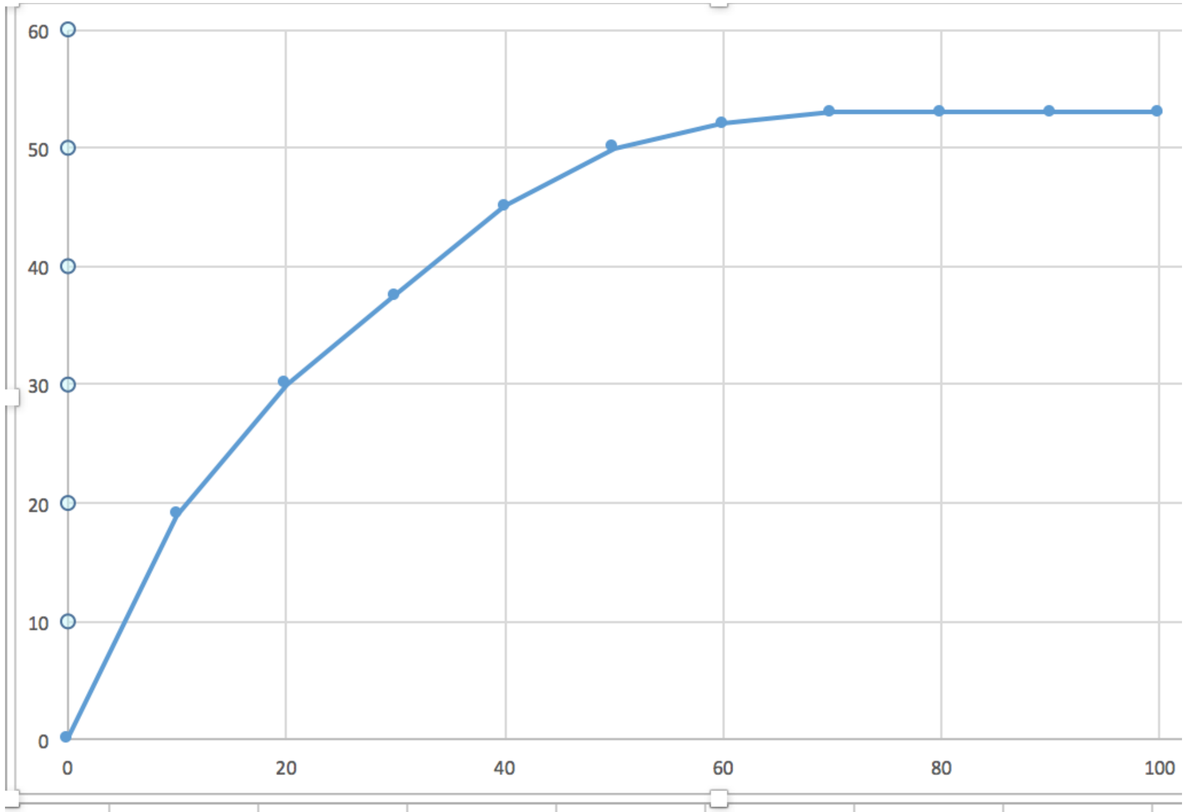
Consider the reaction between limestone and hydrochloric acid

- $CaCO_{3(s)} + 2HCl_{(aq)} \rightarrow CaCl_{2(aq)} + CO_{2(g)} + H_2O_{(l)}$
- This reaction rate can be measured by detecting the amount of Carbon dioxide captured



Data Collection during the chemical reaction

$V[CO_2]$/ cm^3	t/s
0.0	0.0
19.0	10.0
30.0	20.0
37.5	30.0
45.0	40.0
50.0	50.0
52.0	60.0
53.0	70.0
53.0	80.0
53.0	90.0
53.0	100.0



Ways to measure the rate of reaction using a graph

- Average rate
- Instantaneous rate
- Initial rate

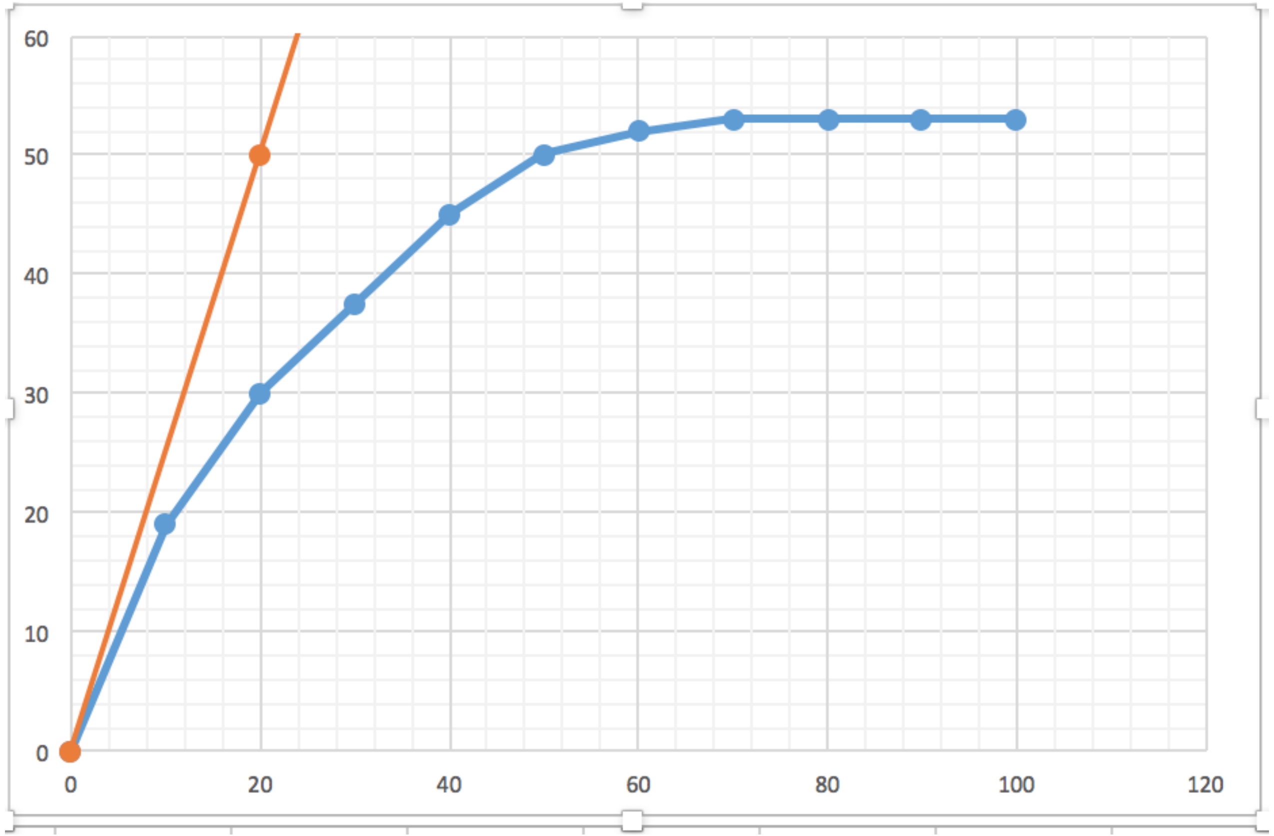
Average Rate

- The average rate is a measure of the change in concentration over time
- $Average\ rate = \frac{\Delta c}{\Delta t}$
  - Δc is the change in concentration
  - Δt is the time interval
- For gases we can say Δc is ΔV
- $Average\ rate = \frac{53.0}{70.0} = 7.57 \times 10^{-1}$ $cm^3\ s^{-1}$

Instantaneous Rate

- $\lim_{\Delta t \to 0} \frac{\Delta c}{\Delta t} = \frac{dc}{dt}$

Initial Rate



- The initial rate is the instantaneous rate at t=0
- A tangent line is drawn from t=0 (red line)
- $Initial\ Rate\ = \frac{\Delta y}{\Delta x} = \frac{50-0}{20-0} = 2.50\ cm^3 s^{-1}$

Rate equation

- Consider the following equation xA + yB → qC + pD
- The rate reaction is a mathematical differential equation that shows how the rate relates to the concentration
- $rate = -\frac{1}{x} \cdot \frac{d[A]}{dt} = -\frac{1}{y} \cdot \frac{d[B]}{dt} = +\frac{1}{p} \cdot \frac{d[C]}{dt} = +\frac{1}{q} \cdot \frac{d[D]}{dt}$

Kinetic Molecular theory of gases

- Explains why gases follow the ideal gas law (pv=nrt)
  - Also call the kinetic theory of gases.

Contains four main ideas:

1. Gases contain many molecules moving at high speeds in random directions
2. The size of the atoms is negligible
3. Collisions between gases are completely elastic and NRG is not lost only transferred
4. The average kinetic NRG is proportional to the temperature in kelvin. Particles are moving at many different velocities.

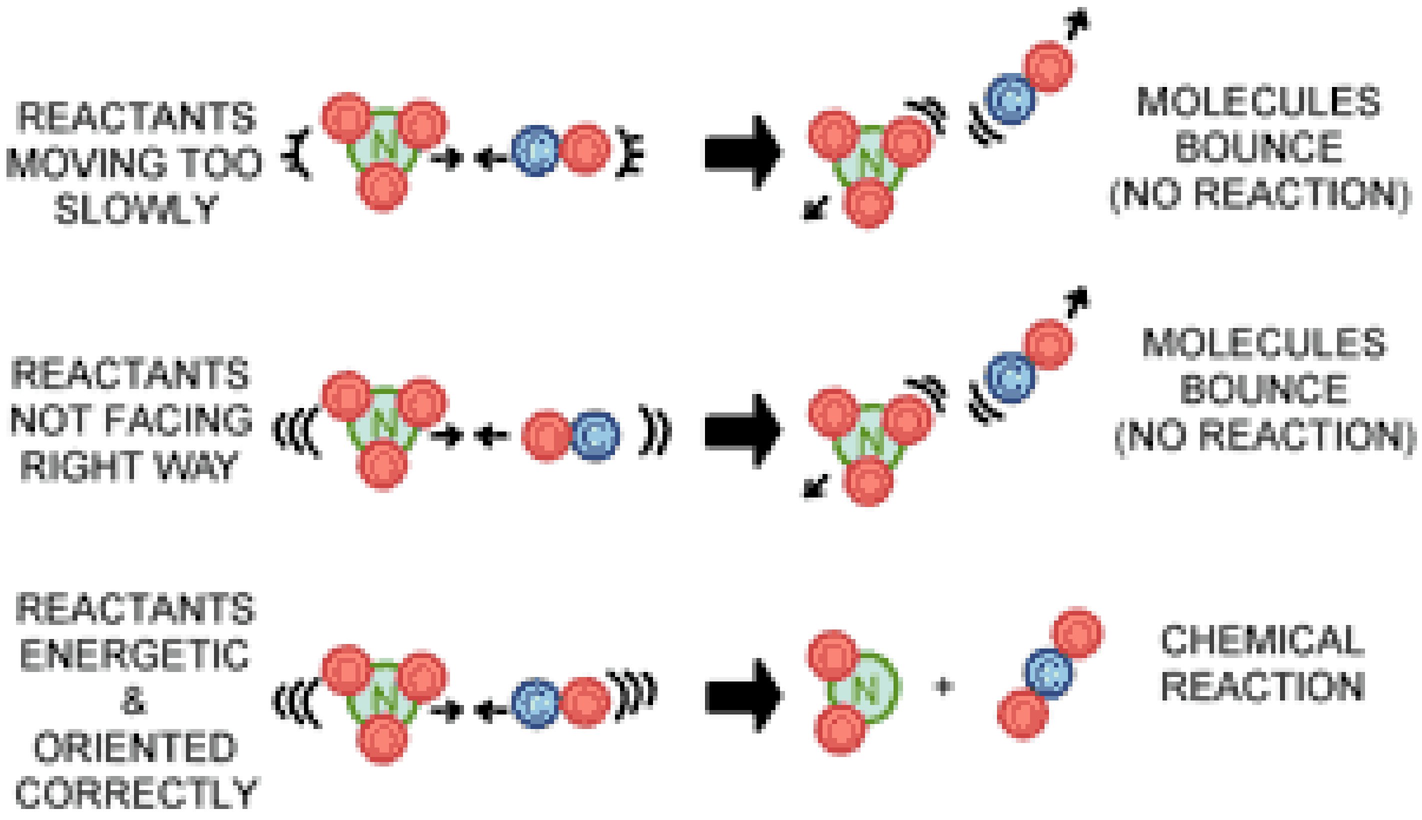
These four postulates can be used to explain temperature and pressure of a gas and thus the ideal gas law can be derived.

Collision Theory

- Created using Occam’s razor (Nature of Science)
  - Occam’s razor is a principle that state’s “Entities should not be multiplied unnecessarily”
  - This principle is used as a guide in the development of theories.
  - Collision theory is one example of this theory in action.

Collision Theory

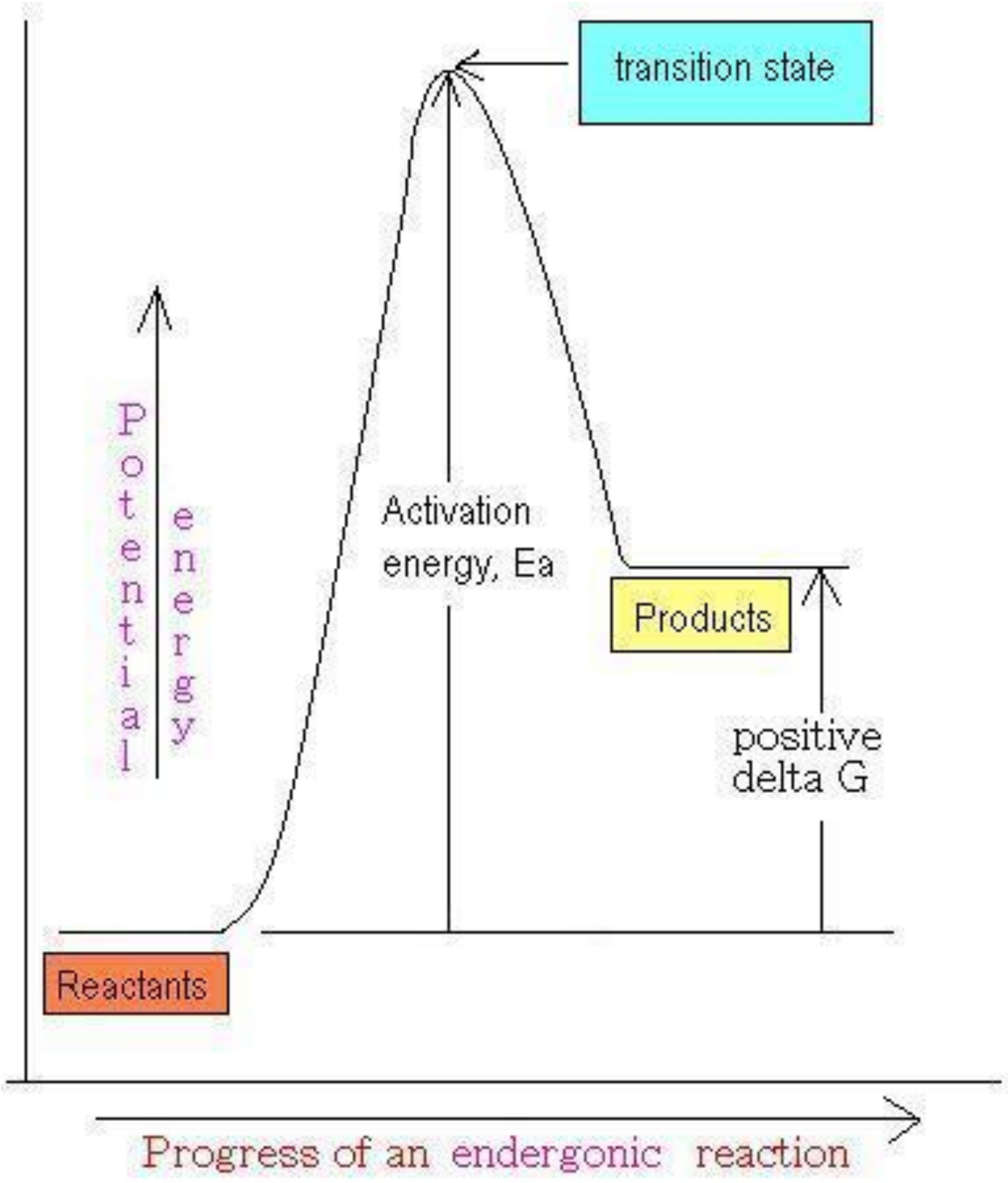
- Collision theory states that for a chemical reaction to occur the following conditions must be met:
  - Two particles must collide
  - Colliding particles have to have the correct orientation
  - They must have enough kinetic NRG to start the reaction
- This based on the kinetic theory of gas
- Explains why temperature influences reaction rates
- Explains why most reactions do not go to completion



REACTANTS MOVING TOO SLOWLY
MOLECULES BOUNCE (NO REACTION)
REACTANTS NOT FACING RIGHT WAY
MOLECULES BOUNCE (NO REACTION)
REACTANTS ENERGETIC & ORIENTED CORRECTLY
CHEMICAL REACTION

Catalyst

- Activation energy is need to start a chemical reaction.
- Its like pushing a rock up hill, once it gets to the top it can roll down to the products.
- This can be shown in a potential energy diagram
- The transition state at the top can be called an activated complex as well.
- Lower the activation NRG so its easier to start the reactions



Catalyst

- There are two types of catalyst: Homogeneous and Heterogeneous
- Homogenous catalyst are catalyst that are in the same physical state as the reactants.
  - Ex. Destruction of ozone by chlorine atoms
- Heterogeneous catalyst are catalysts in a different state from the reactants.
  - Generally the catalysts are solids and the reactants are liquids and gases.
  - Ex. Catalytic converted in cars to help decrease dangerous gases realeased by the combustion of gasoline.

Maxwell-Boltzmann energy distribution and temperature

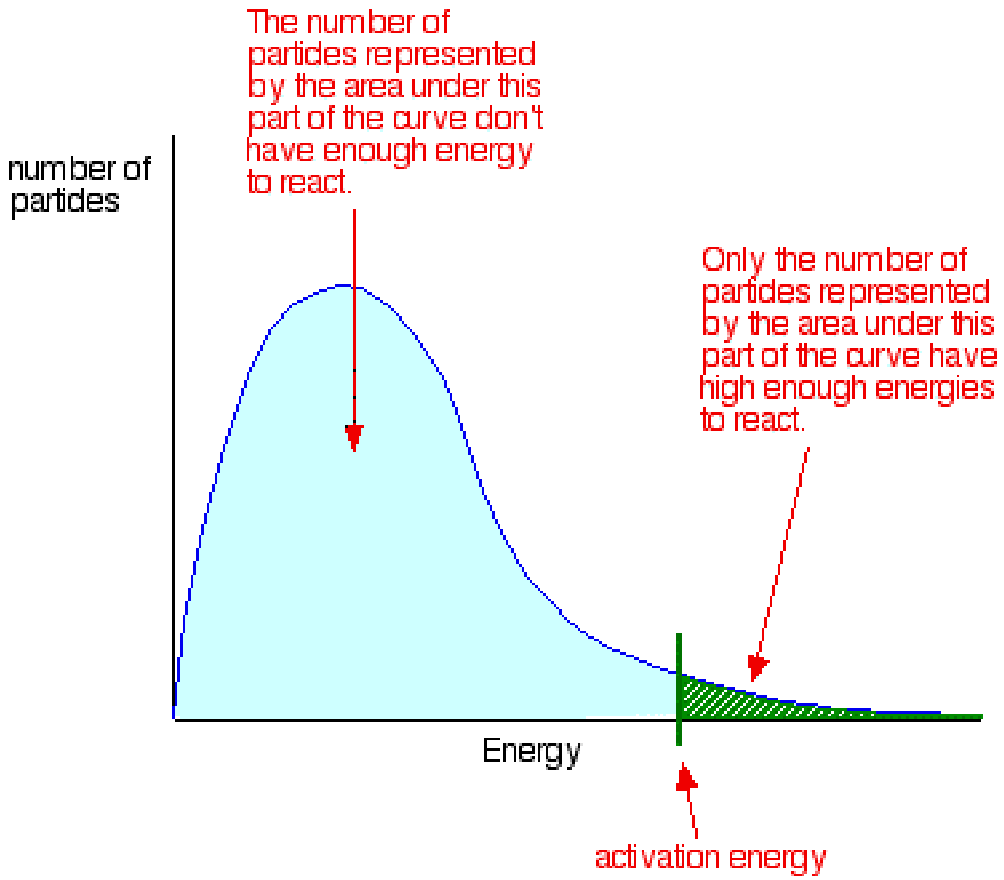
- Rates of reactions in the gas phase can be interpreted at the molecular level using
  - Collision theory
  - Temperature effects on Kinetic NRG
  - Maxwell-Boltzmann energy distribution curves

Maxwell-Boltzmann energy distribution and temperature

- The kinetic theory tells us that gases are always moving randomly and at high velocities.
- These velocities are different (temp is only the average) and always colliding, thus changing directions.
- Therefore, it doesn’t make sense to talk about each molecule’s energy independently. Instead we consider their distributions.

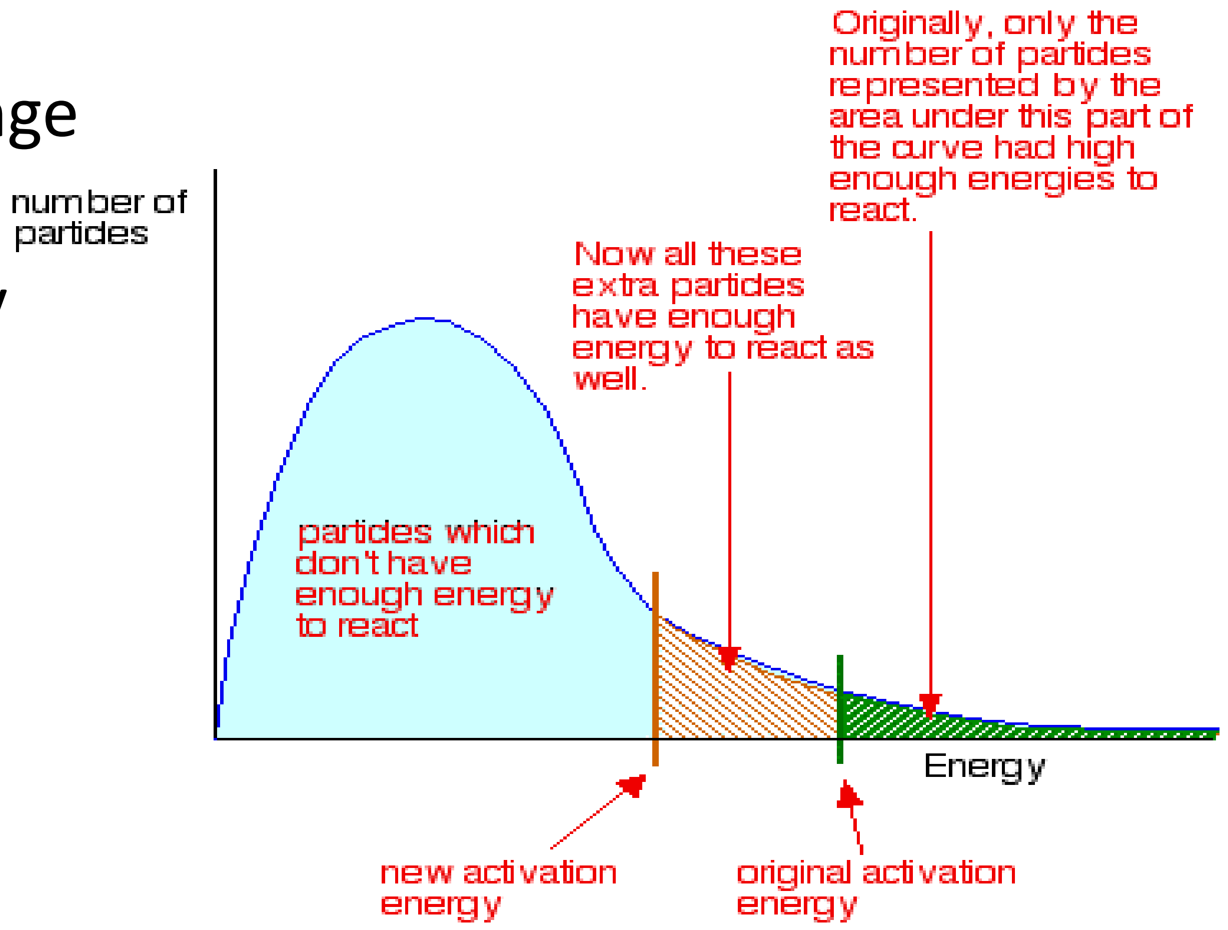
Maxwell-Boltzmann energy distribution curve

- These charts can show us how many particles have enough energy to overcome the activation energy of a reaction
- The area under the curve represents the number of atoms that can or can not react
- Most atoms are near the mean of the kinetic energy (near the hump)



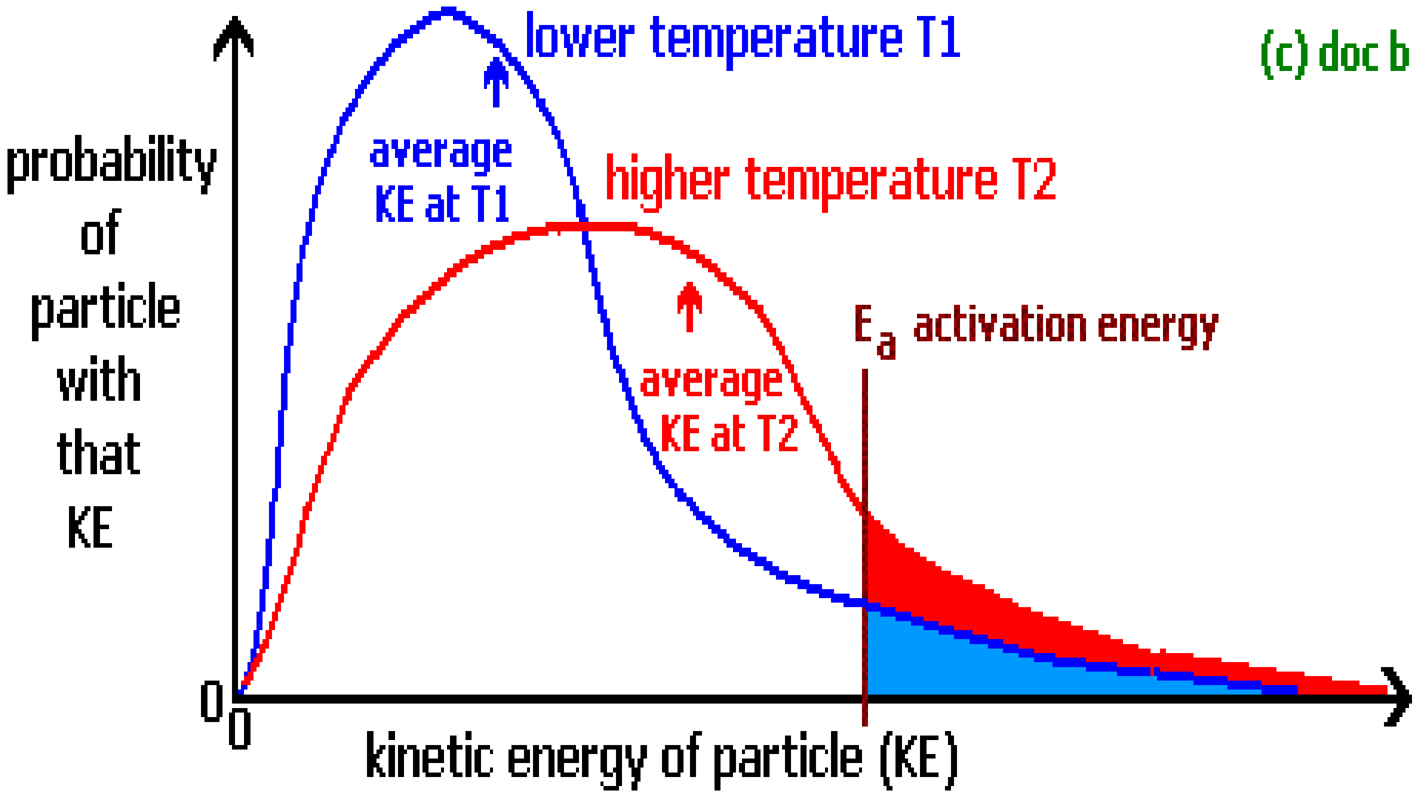
Maxwell-Boltzmann energy distribution curve after a catalyst was added

- The distribution doesn't change
- The number of particles increases because the energy needed is lowered.



Maxwell-Boltzmann energy distribution curve after a catalyst was added

- The distribution changes
- Increasing temperature increase the amount of atoms with enough energy to undergo the reaction.
- As T increase so does particle speed and thus kinetic energy of the gas particles increase and the amount of collisions



Factors that effect the rate of a chemical reaction

1. Increasing the temperature-decreasing temperature can decrease the rate of reaction this is why we put food in the refrigerator
2. Adding a catalyst
3. Increasing the concentration of the reactants- increasing the amount of particles, while keeping the volume the same, will increase the amount of collisions
4. Decreasing particle size of a solid reactant – if you break a solid into smaller pieces, increasing the surface area, you can increase the amount of collisions

Measuring the rate of the reaction

1. Change in pH – use a pH meter and probe to measure the change in pH during an acid base reaction
2. Change in conductivity- Using a conductivity probe and meter you can measure the change in ion concentration during an electrolytes reaction
3. Change in mass or volume
4. Change in color- colorimetry is used to monitor chemical reaction that have a colored
5. product.