Picturing Equilibrium

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1 Abstract

Every chemical *reaction* combines component *reactants* to form resulting *products*. In certain cases, and under certain quantities of reactants, the amount of products and reactants being made is in equilibrium. This means that is the rate at which products are being made equals the rate at whcih reactants are being made.

This project demonstrates the effects of chemical equilibrium and explaining the reasoning and conditions behind it. This will be accomplished by creating a model using VPython and pairing them with explanations.

2 Background

Chemical *equilibrium*, by definition, is the state in which the reactant and products of a chemical reaction have no net change over time.

2.1 Types of Equilibrium

There are two types of equilibrium, *static* and *dynamic*.

- *Static equilibrium* occurs when a chemical reaction is *irreversible*. That is, reactants may only be made into products. Since at completion, the rate of the forward reaction, or the reactants being made into products, and backward reaction, or the products being made in reactants is 0, and thereby equal to one another, static equilbrium is a type of equilibrium.
- *Dynamic equilibrium* occurs when a chemical reaction is *reversible*. That is, reactants are made into products but products can be reversely made into reactants. The equilibrium point is achieved when the rate of product production equals the rate of reactant production. We will be focusing on dynamic equilibrium in this project.

2.2 Chemical Equations

A chemical equation differs from a mathematical equation in that it does not contain an equal sign, but an arrow instead. In an equilibrium system, it is a double sided arrow. The arrow/double sided arrows stands for the word, produces. The chemical equation written below displays a standard chemical equation rewritten by variables.

$$aA + bB \longleftrightarrow cC + dD$$

The lowercase letters stand for the amount of compound being used in the reaction in units of *moles*. A mole is defined as

$$6.022 * 10^{23}$$

units of substance. In chemistry, these units of substance are molecules.. The uppercase letters stand for the compounds in equilibrium. Thoses on the left, A and B are the reactants. On the right you have the products C and D.

For example, take the chemical equation:

$$H_2 + I_2 \longleftrightarrow 2\,HI$$

In the situation, using the defined variables above, A is synomous with H_2, B is synomous with I_2, C is synomous with HI, a =b=1, and c=2. Notice that even though there is no value directly corresponding with the position of a or b, we can assume it is one, because in standard notation, chemists do not write out the coeffficient if it is one. Also, notice that D and d do not exist in the chemical equation involving HI. You only need to assign variables to the compounds in the chemical reaction. Since there is no fourth component to the reaction, we do not need to use the variable D or d.

2.3 Dynamic Equilibrium

The concept of dynamic chemical equilibrium was first proposed when Claude Louis Berthollet discovered that some chemical reactions are reversible in 1803. From there it was found that many reactions produced both reactants and prodcuts at the same time. Further analysis revealed that every reaction has a unique constant associated with it.

2.4 Reaction Quotient

The reaction quotient is a constant that tell us the ratio of products to reactants at a specific state in the reaction. It is determined by the equation below.

$$\frac{[C]^c[D]^d}{[A]^a[B]^b} = Q_c$$

The elements within the brackets symbolizes the concentration of those compounds in units of molarity, which is the amount of moles of substance divided by the amount of liters it is contained in.

2.5 Equilibrium Constants

An *equilibrium constant* tells us the ratio of products to reactants at a reaction's equilibrium state. Every single equilibrium reaction has it's own equilibrium constant. This can be found experimentally by determining the concentrations of all the substances when you know the system is in equilibrium.

For example, the equilibrium system $N_2 + 3\,H_2 \longleftrightarrow 2\,NH_3$ has a unique constant of 152. But the equilibrium system $CO_2) + H_2 \longleftrightarrow CO + H_2O$ has a unique constant of 0.64.

- If K (the equilibrium constant) is greater than 1, then equilibrium favors products. That means, that in the equilibrium state, there will be more products then reactants.
- If K is less than 1, then equilibrium favors reactants. That means in the equilibirum state of the reaction, there will be more products than reactants.

Comparing the reaction quotient and equilibrium constant tells you how the system will behave.

- When Q_c=K the system is at equilibrium.
- When Q_c does not equal K, the system is not at equilibrium and will produce more products or reactants to achieve equilibrium.

2.6 Le Chatelier's Principle

Le Chatelier's Principle is a set of laws devised by chemist Henry Louis Le Chatelier in 1884 in order to predict the effects to an equlbrium system when subjected to change in temperature, concentration, pressure, or volume.

Concentration

- If you increase the concentration of a reactant in a equilibrium system, the system will create more products to bring the increased reactant concentration back down. In technical terms, the equilibirum *shifts* towards the reactants.
- If you increase the concentration of a product in a equilibrium system, the system will shift towards the reactants.

Temperature

- If heat is added and the reaction is *exothermic* (heat is a product), then the equilibrium system will create more reactants to bring the temperature back down.
- If heat is added and the reaction is *endothermic* (heat is a reactant) then the equilibrium will shift towards the products.

Pressure

- If pressure is decreased suddenly (say the volume of the container of gases was replaced with a larger one), then the equilibrium will shift towards which side produces the most total moles of substance.
- If pressure is increased suddenly (say the volume of the container of gases decreased), then the equilibirum will shift towards which side produced the least total moles of compound.
- It should be noted that anything that changes total pressure of the system will not affect the equilibrium constant. For example, adding another gas which adds to the total pressure of the system doesn not affect anything. When you change the container of the reaction, you are in fact changing the partial pressure all of the gases.

3 Goals

The goals for this project is to:

- Create one 3D animation of an equilibirum system demostrating what happens when one of the three conditions (either temperature, volume or concentration) are changed according to Le Chatelier's Principle.
- Create a website with detailed explainations of this principle.

3.1 Methods

I'm going to do this project by studying and annotating the VPYthon example "gas.py", and making modifications and renovating parts of it in order to demostrate chemical equilibrium.

3.2 Timeline

By 11/06/2015, I will have two seperate elements in the model.

By 11/13/2015, I will make all the atoms collide with each other and some will stick together. I will also have presented my seminar at this point.

By 11/20/2015, I will make the atoms be able to seperate at random velocities after a certain time interval.

By 11/30/2015 I will finish the animation and will finish the website as well.