Picturing Equilibrium

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1 Abstract

Equilibrium is a concept that is applied throughout all of the natural world. Every chemical reaction that occurs ends at its equilibrium state. However, visualizing this concept is difficult when you are exposed to it for the first time. Some reactions seem like they end leaving only products, but when examined further it is seen that there in fact there is a little bit of reactants left.

This project is aimed at demonstrating the effects of chemical equilibrium and explaining the reasoning and conditions behind this event. This is hoped to be accomplished by creating a model/models using Python/VPython and pairing them with explanations. The first section will outline the mathematics/chemistry behind equilibrium, and the second section will outline the goals of this project.

2 Background

Equilibrium, by definition, is the state where the rate of product production equals the rate of reactant production. In order to work with the mathematics behind equilibrium, the first step is to write the equilibrium equation.

The first step is to rewrite the chemical equation in that is being analyzed.

aA + bB $\longleftrightarrow$ cC + dD

This transforms the parts of a chemical equation into variables we can use to represent an equilibrium equation. The bolded variables are the coefficients of the compounds/elements being used, and the uppercase letters stand for the compounds/elements.

The equlibrium expression for concentrations is written as:

$$([C]^c[D]^d)/([A]^a[B]^b) = K_c$$

To clarify, the variables [A],[B],[C] and [D] in this equation represent the molarities of the aqueous and gaseous compounds. Solids are not represented in the equlibirum expression. The variables a,b,c, and d are the coeffiecients of the compounds in the equation.

We have a very similar equation for equilibrium of pressure. This is written as:

$$(P_C^c)(P_D^d)/(P_A^a)(P_B^b) = K_p$$

Here, partial pressure of gases are used instead of concentrations, but the basic concept is still the same.

The solution to those equations is what we know as the equilibrium constant.

The equilibrium constant in essence is a ratio of concentrations of products over reactants. There are a couple general truths that apply to both pressure equilibrium and concentration equilibrium.

- If K is greater than 1, then equilibrium favors products. That means, at that moment in time, more products are "wanting" to be made than reactants.
- If K is less than 1, then equilibrium favors reactants. That means, at that moment in time, more reacctants are "wanting" to be made than products.

But in general chemistry, the concept usually to be tested is equilibrium shifts. In those problems, a equation is given and an outside modification is made. Students are expected to be able to identify where the equilibrium has shifted to at that time and whether more products are reactants will be made.

For example given this chemical equation:

$$H_2(g) + O_2(g) <-> H_2O(l)$$

And told 5 L of oxygen were added to the equilibrium system, students would be asked to predict which direction the equalibrium would shift to maintain equilibrium. In this case we would apply a concept called Le Chatelier's Principle.

Le Chatelier's Principle is merely a set of "laws" that we can apply to situations such as this to determine the shift in equilibrium.

Concentration

- Changing the concentration of a chemical shifts the equilibrium to the side of the reaction that would reduce that change in concentration.

Temperature

- If heat is added and the reaction is exothermic (heat is a product), then the equilibrium will shift towards the reactants.
- 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 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 moles of substance.
- 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 minimum goals for this project is to:

- Construct a working/inputable model of equilibrium that demostrates the effects of Le Chatelier's Principles using Python/VPython.
- Create a website with detailed explainations of this principle.

The extra goals to be achieved after the minimum are:

- Incorperate the equilibrium equations into the model and be able to link the model with the change in the equations.