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Thermodynamics and chemical kinetics go hand in hand

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Abstract
The results of this study indicate that thermodynamics and reaction kinetics, two major fields within chemistry, are connected by various reactions, and are both necessary to understand in connection in order to get a favorable result. These include the reactions of acid dissociation, the Haber process, and the formation of water, which are the three reactions covered within this study.

Keywords: Thermodynamics, dissociation, collisionfrequency, Enthalpy, activation energy, entropy, chemical equilibrium, Gibbsfreeenergy

Introduction

Yash Raj Mehta, a student of A level from DPS International, Saket, New Delhi, has been an activist in My Right to Breathe and anti-pollution activities. In class 6th, he went to Gazipur landfill himself to make a project and has been vocal about anti-smog, garbage disposal, and its threats to our lives. He has participated in many protests at a very young age, and feel a sense of responsibility towards our society and country by proposing doable solutions through his write ups and talks in school. A chemical engineer aspirant and blue coat scholar badge holder, Yash Raj, loves nature and marine world. He strongly believes that we all are deeply connected and taking care of our natural resources is our collective responsibility. This study was done under the supervision of Dr. Imran Khan.

Chemical equilibrium

The state in which both the reactants and products are present in concentrations which have no further tendency to change with time.

Gibbs free energy: a thermodynamic potential that can be used to calculate the maximum amount of work, other than pressure-volume work, that may be performed by a thermodynamically closed system at constant temperature andpressure.

Example 1: Acid dissociation

The strength of an acid is dependent upon its degree of dissociation in water, meaning the proportion of hydrogen that leaves as ions in the water.

A weak acid dissociates partially, whereas a strong acid dissociates completely.

Stronger acids have a lower pH. The pH of an acid can be calculated via the formula:

$$pH = -log[H_3O^+]$$

This formula yields the pH of ethanoic acid-a weak acid- to be roughly 3.0, and the pH of Hydrochloric acid- a strong acid- to be roughly 1.1. These values correspond with their respective dissociation equations.

$$CH_3COOH\ (aq) \rightleftharpoons H^+(aq) + CH_3COO^-(aq)$$
$$HCl(aq) \rightarrow H+(aq) + Cl-(aq)$$

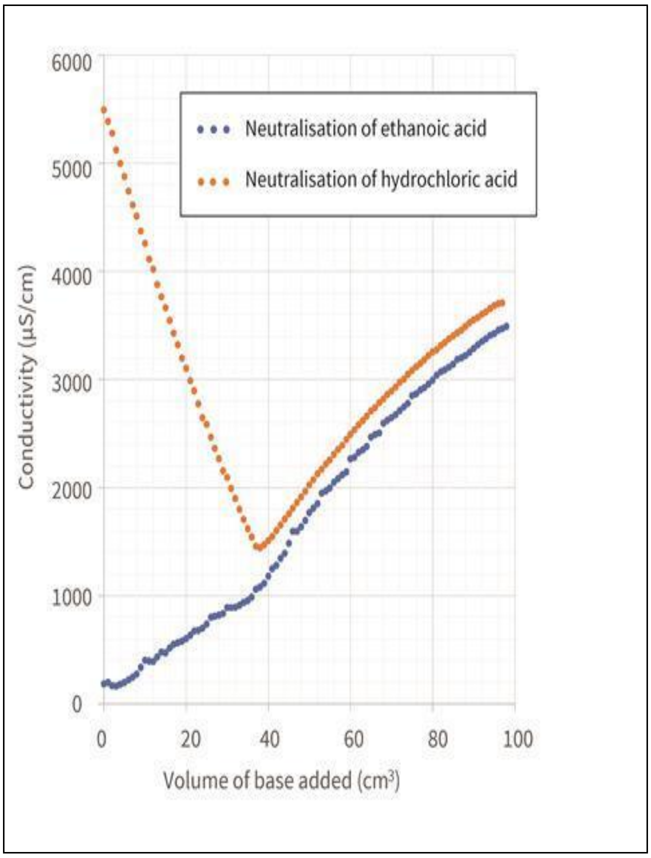
The rate of reaction for either reaction can be calculated via calculating the conductivity of the solution over time, using a conductivity meter. This conductivity increases as the number of ions-the products- increases in the solution. Conductivity is measured with a probe and a meter. Voltage is applied between two electrodes in a probe immersed in the solution. The drop in voltage caused by the resistance of the solution is used to calculate the conductivity per centimeter. The meter converts the probe measurement to micromhos per centimeter and displays the result for the user. The total dissolved solids concentration in milligrams per liter (mg/L) can also be calculated by multiplying the conductivity result by a factor between 0.55 and 0.9, which is empirically determined.

As stronger acids are more willing to dissociate, they have a higher rate of reaction, and thus the conductivity increases more quickly as the aqueous hydrochloric acid dissociates. The enthalpy change of a reaction can be calculated using theformula:

$$\Delta H = \text{Energy into the reaction} - \text{Energy out of the reaction}$$

Weaker acids have a greater enthalpy change. As they tend less to dissociate, extra energy is needed to ionize the molecules. Since no bonds are formed, the energy out of the reaction remains the same.

Similarly, stronger acids have a lower enthalpy change, as the acid is more willing to dissociate and doesn’t require as much energy to ionize.



Neutralization of ethanoic acid vs hydrochloric acid

Example2: The Haber process

The Haber's process is an example of a reversible reaction, wherein the reaction system reaches equilibrium, a state in which the forward reaction and the reverse reaction occur at an equal rate, and the concentrations of neither the reactants nor the products change.

Eq. for Haber's process:

$N_{2}(g)+3H_2(g)\rightleftharpoons 2NH_3(g)\ \Delta H=-92.4\ kJmol-1$

The forward reaction is exothermic, and thus the backward reaction is endothermic, with a standard enthalpy change of *$\Delta H=+92.4kJmol-1$*.

This reaction is done to industrially produce ammonia, which is used in the creation of fertilizers, such as ammonium nitrate (NH_4NO_3).

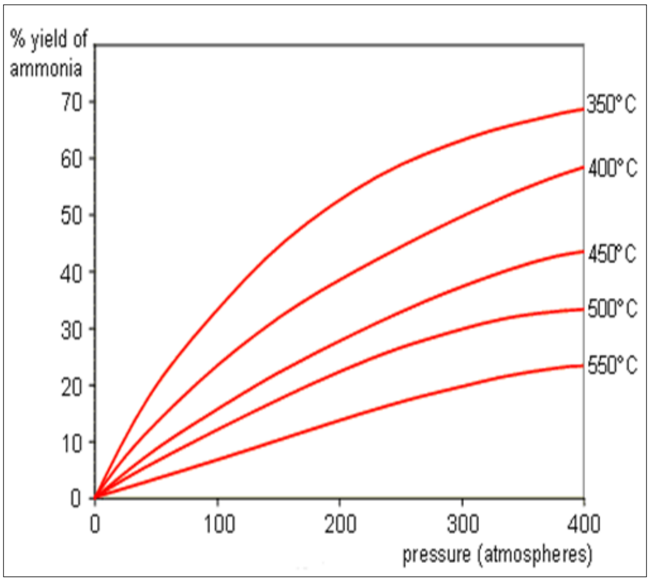
As an industrial process, the main aim is to quicken the production of ammonia, while also making sure a favorable. yield is produced, by shifting the position of equilibrium using external factors. This abides by Lee Chatelier's principle.

As the aim is to improve the yield of ammonia, while also keeping a steady rate, the variables of the experiment need to be adjusted accordingly. Increasing the temperature increases the rate of both the forward and reverse reactions, as according to kinetic theory, a greater proportion of the molecules of both sides would have sufficient activation energy to engage in successful collisions

However, increasing the temperature also affects the yield. Increasing the temperature doesn't equally favour both reactions, it mainly favors the endothermic reaction, i.e. the backward reaction. This is the reaction wherein there is a net energy surplus. Thus, the rate of decomposition of ammonia increases by a greater margin than that of the reaction of nitrogen and hydrogen. This causes equilibrium to shift toward the left, decreasing the yield of ammonia. On the other hand, decreasing the temperature would increase the yield of ammonia, while decreasing the rate of reaction. A decrease in temperature causes the rate of the endothermic reaction to decrease by a greater margin than that of the exothermic reaction, which shifts equilibrium to the right.

Due to these constraints, there lies a trade-off. Increasing the temperature would certainly increase the rate of reaction, which is favorable, but would also decrease the yield of ammonia. Reducing the temperature would improve the yield of ammonia, but the process would slow down, which is unfavorable as more time would be taken to produce unit product.

Hence, a balanced temperature is chosen, 450 degrees Celsius



Variation of yield of ammonia with different temperatures with certain pressure values

Example 3: Reaction of hydrogen and water

The balanced chemical equation for the combustion of hydrogen is:

$2H_2(g) + O_2(g) \rightarrow 2H_2O(g)$

This reaction involves both thermodynamic and kinetic aspects:

Thermodynamics

The reaction is exothermic, meaning it releases heat energy to the surroundings. This is indicated by the negative enthalpy change (ΔH) associated with the reaction.

The reaction is also accompanied by a decrease in entropy (ΔS), as the number of gaseous molecules decreases from three (H2 and O2) to two (H2O). This decrease in entropy favors the forward reaction.

The Gibbs free energy change (ΔG) for the reaction determines whether the reaction is spontaneous or not. For an exothermic reaction like this, with a negative ΔH and a decrease in entropy (ΔS), ΔG will be negative at temperatures below the equilibrium temperature, indicating that the reaction is thermodynamically favorable.

Kinetics

The rate at which the reaction occurs depends on the collision frequency of hydrogen and oxygen molecules, as well as the activation energy required for the reaction to proceed.

Catalysts, such as platinum or nickel, can be used to increase the rate of the reaction by providing an alternative pathway with a lower activation energy.

The reaction rate can also be affected by factors such as temperature, pressure, and the presence of inhibitors.

By considering both the thermodynamic and kinetic aspects of the reaction, we can gain a comprehensive understanding of its behavior, including whether it will occur spontaneously and at what rate.

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