Conditions for the haber process

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In this essay I will find out what are the best conditions for the production of the maximum yield in the Haber process, by running simulations of the Haber process at different conditions to determine the best conditions. From the Experiment I found that the lowest temperature possible and the highest pressure possible would provide the best conditions to operate the Haber process at for the maximum yield possible.

Introduction

The Haber process is an important Process used in chemical Industry to manufacture Ammonia from Nitrogen and Hydrogen that originate in the air. The reason why it's very important is it turns an inert gas Nitrogen (N2) and a very volatile and reactive gas Hydrogen (H2) into ammonia which is a stable compound but reactive enough to be used in different aspects.

Why was the Haber process discovered?

During the First World War " Britain Cut off Germany Supply route to Chiles salt peter natural deposits". Since the Allies (" Russian Empire, United Kingdom, France, Canada, Australia, Italy, the Empire of Japan, Portugal and the United States") has gained control over the natural deposits of saltpetre from natural deposits found in Chile, therefore cutting off Germanys access to materials that the needed to produce necessary items such as food, guns, bombs other war materials. Germany has to find ways to produce its own hence the Haber process which was discovered in 1909 by a German chemist named Fritz Haber to produce ammonia was set into industrial scale in 1913; the produced ammonia was later processed into a Synthetic Form of Chile saltpetre

Introduction

The Haber process is the process that uses extracted nitrogen from the atmosphere and reacts the nitrogen (N2) gas would react with 3 moles of hydrogen (H2) gas by using a medium temperature around 473K-673K (200-400°C) High atmospheric pressures such as 250 atmospheres (25331250 Pascal) and a catalyst to create ammonia (NH3). Due to advancements made to technology we are able to do reaction at extremely high temperatures such as 2300K (2026°C) and we know that a reaction occurs faster when conducted at the highest temperature possible but the Haber process's success is not calculated on the speed of the reaction but on the yield of the ammonia that is produced during the reaction. Although increasing the temperate would surly increase the rate of reaction in a normal forward reaction the problem with using this method on the Haber process is it's not a normal forward reaction type of reaction but is an equilibrium type of reaction.

The Chatelier's Principle states increasing the temperature will cause the equilibrium position to shift to the left side of the reaction resulting in a lower yield of ammonia because the forward reaction is exothermic.

N2(g)

nitrogen

+

3H2(g)

hydrogen

Very High heat, Low pressure, catalyst

$2NH_3(g)$

ammonia

Reducing the temperature will cause the equilibrium system to change the point of equilibrium to minimise the effect of the change, and hence it will produce more heat due to an increase the exothermic reaction therefore causing the wanted increase in the yield of ammonia.

$N_2(g)$

nitrogen

+

$3H_2(g)$

hydrogen

Low heat, High pressure, catalyst

$2NH_3(g)$

ammonia

However, the rate of the reaction at very lower temperatures is exceptionally slow, and so a higher temperature should be used to increase the speed of the reaction which results in a lower yield of ammonia but a temperature low enough to create more ammonia than use in the reverse reaction hence we have the final equation is an which an above normal ammonia production.

$N_2(g)$

nitrogen

+

$3H_2(g)$

hydrogen

High Temperature, Low pressure, catalyst

http://www. avogadro. co. uk/chemeqm/eqm_sign. gif

$2NH_3(g)$

ammonia

Increasing the pressure condition of the haber chamber causes the equilibrium position to shift to the right resulting in an increased yield of ammonia because ammonia has more gas molecules (more moles) on the left hand side or the forward reaction of the equation (4 in total 3 Hydrogen and 1 Nitrogen) than there are on the right hand side or backwards reaction of the equation (2 in total $2NH_3$).

$N_2(g)$

nitrogen

+

$3H_2(g)$

hydrogen

High Temperature, Low pressure, catalyst

$2NH_3(g)$

ammonia

Increasing the pressure means the system will have to adjust to reduce the effect of the change, which is reducing the pressure built up by reducing the amount of moles that can be located in the equilibrium reaction.

Uses as ammonia

One of nitrogen's upper most important uses is in making ammonia (NH_3), which is a colourless gas with a strong odour, similar to the smell of urine because urine contain some most definitely contains ammonia.

The production of ammonia changes the non oxidation properties of nitrogen as the Oxidation reaction.

Pharmaceuticals

" Used in the manufacture of drugs such as sulphonamide" which " inhibit the growth and multiplication of bacteria" buy the removal of replacing the " aminobenzoic acid for the synthesis of folic acids and minerals as well as vitamins and thiamine".

Fertilizer

An important usage of ammonia is in the making of fertilizers. " Ammonia can be used directly as fertilizer by adding it to irrigation water" because plants need a good supply of nitrogen in order to grow and which ammonia is able to provide. It is also used to produce the urea (NH2CONH2), which is also used as a fertilizer. Another important use of ammonia is to create nitric acid (HNO3), which is then also used to make fertilizer. The Haber Process didn’t lonely provide the Germans with Saltpetre but revolutionized the agriculture industry with an increased yield in crop production enabling them to continue.

Cleaning Products

“ Many people use household ammonia as a disinfectant. Nitric acid-made form ammonia-is used in explosives. Ammonia is also used in the plastic industry and as a feed supplement for livestock”.

The dipole moment of this compound and this is consistent with its geometry, a triangular pyramid due to it’s electronic arrangement obeying the octet rule, Four pairs of electrons three bonding pairs and one lone pair repel each other giving the molecule the triangular pyramid shape of bond angles of 107 degrees is close to the tetrahedral angle of 109. 5 degrees. The electronic arrangement of the valence electrons in nitrogen is described as sp3 hybridization of atomic orbitals.

The NH3 molecules and their ability to make hyrodgen bonds explains thir polarity and high solubility of ammonia in water. A chemical reaction occurs when ammonia dissolues in water as it acts as a base acquiring a hydrogen ion from H2O to ammonium and hydroxides ions

NH3(aq) + H2O(l) http://www. avogadro. co. uk/chemeqm/eqm_sign. gif NH4+(aq) + OH-(aq)

The production of hydroxide ions when ammonia dissolves in water gives the solution of ammonia it's alkaline characteristics (basic properties), The double arrow in the equation states that an equilibrium has been reached between the dissolved ammonia gas and ammonium ions

The ammonium ion acts as a weak acid aqueous solution because it dissociates to form Hydrogen ion and ammonia. (Shakhashiri, 2008) This is why dissolved ammonia is used in cleaning products because it's able to react with both and acid stain and alkaline stain meaning it's an all round cleaning products even though the acid is weak it's strong enough to deal with domestic stains.

Explosives

Sodium Nitrate is a Chemical compound with the chemical compound of NaNo3 has been referred to as Chile saltpetre before. And is produced by a reaction of a metal and an acid to produce a salt and is highly soluble in water. (Quote)

Sodium Nitrate can be used as a fertilizer and as a material from the production of explosive gunpowder. Naturally gun powder is a rapid burning compound made of Carbon (C12) potassium nitrate, KNO3 and Sulfur and is used in guns because of its capacity to burn in a rapidly producing enough pressure to propel a bullet and not explode. (Quote)

Sodium nitrate has " antimicrobial properties" when used as a food preservative. It can be used in the production of nitric acid by combining it with sulfuric acid. It can used as a substitute oxidizer used in fireworks as a replacement for potassium nitrate commonly found in gun powder. Because sodium nitrate can be used as a Phase Change Material it may be used for heat transfer in solar power plants.

Imporantance of Nitrogen

Nitrogen gas (N2) is often used as a substitution for air which is a mixture of 78% nitrogen 78%), Oxygen 20%, and 1% of other gases such as Water Vapour Argon and Carbon dioxide (0. 03%). where oxidation is unwanted. One area for use is to maintain the freshness to food products by packaging them in nitrogen gas to reduce the fermenting of food due to its properties for preventing oxidization which can cause Rancid “ unpleasant odour or taste of decomposing oils or fats” (http://www. school-for-champions. com/chemistry/nitrogen_uses. htm). Argon has been used as replacement for air in light bulbs to prevent the heated tungsten filament from reacting with the oxygen found in air because Argon is an inert gas but is expensive so ammonia can be reverted back to Nitrogen gas by the process gentrification to replace Argon in light bulbs and is cheaper inert material than Argon.

Nitrogen is also used as a controlled storage and Transportation measure food packages due to it’s capacities to be used as a noble gas, to extend the shelf life of fruits and vegetables and is “ now used during storage to displace most of the oxygen in the containers” http://www. igs-global. com/nitroswing/hdlg. htm, for the purpose of slowing down the reparation and deterioration of food as proven in biochemistry as in aerobic respiration 32 ATP molecules are created from one glucose molecules and 2 ATP molecules are created from one glucose molecule which is a clear sign that respiration and deterioration of food occurs at 16 times slower during anaerobic respiration which respiration without the presence of oxygen, than respiration occurring aerobically which is respiration with oxygen present.

Investigation

Design

To do this Investigation I will be using a simulator that allow we to change the conditions of the Haber process chamber and notice the change in the yield and work out the direction that the equiliburm will take with extra options such as catalysis.

Firstly I had to decide what the 2 variables I would be looking at during this investigation and decided that the dependant variable will be the yield of ammonia that I would receive from running the simulations.

The Controlled variable will be the temperature and atmospheric pressure that the reaction will be taking place. Another variable that I looked at was if the reaction will be taking place in the presence of a catalyst of not. It was decide that due to the lack of acquiring two or more simulations that were able to run the haber process reaction in the presence of a catalyst

The uncontrolled variable would be required in this reaction because the aim of the reaction is to achieve a dynamic equilibrium which is a reaction in which the forward reaction and backward reaction are equal in a closed environment. Meaning all variables and atoms present are controlled and accounted for.

Set both simulations at the same pressure and temperature to and begin the reaction recorded both results and create a table of results and find the mean of both tables. Redo the experiment changing the controlled variables every time and recording the yield of the reaction at those conditions

Create a Graph using both the mean table to display the results that where shown in the table.

This Is the haber process taking place without the presence of an iron catalyst at the temperature of 300oC and 191 atmospheric pressure. Which will give me the amount of ammonia produced in grams and will be working out in percentage of the nitrogen used to allow compatibility of the 2 different simulations that one will be using.

Is the Haber process taking place without the presence of an iron catalyst at the temperature that the Chatelier’s Principle indicates will be the most effective in the promotion of increasing the Yield. Because this Simulation cannot give the yield of the Haber process ammonia moles or grams I have to change the data received from the first simulation into compatible data.

Results

From these results obtained in the diagram above we notice an increase in yield as we increase the pressure of the reaction while keeping the temperature the same which agrees with the information placed in the beginning of the introduction which states icreasing the pressure will cause the equilibrium position to shift to the right side of the reaction resulting in an increased yield of ammonia since there are more gas molecules

Simulation 2 (changing the Pressure but keeping the Temperature at 150)

From these results obtained in the diagram above we notice an increase in yield as we increase the pressure of the reaction while keeping the temperature the same which agrees with the information placed in the beginning of the introduction which states the Chatelier's Principle states increasing the temperature will cause the equilibrium position to shift to the left side of the reaction resulting in a lower yield of ammonia because the forward reaction is exothermic.

And the 0. 8 (r) shows that there is a high positive correlation between the yield amount

The Curve tends to show that if the pressure was increased any more that 1000 the increment in the production of ammonia may not be justified for the amount of effort that will be put into creating a haber process camber at that atmospheric pressure.

The equilibrium expression for this reaction is:

Keq =

[NH3]2

[N2][H2]3

Temperature (oC)

Keq

25

6. 4 x 102

200

4. 4 x 10-1

300

4. 3 x 10-3

400

1. 6 x 10-4

500

1. 5 x 10-5

“ As the temperature of increases, the equilibrium constant decreases as the yield of the ammonia decreases”. http://nawabi. de/chemical/ammonia. asp

The results of the Ka test agree with the graphs that simulation 1 and simulation 2 provided. As the Ka increases the PH reduces towards the more acidic range meaning the NH3 concentration increases meaning for the best yield of the Haber process, industry must obtain the highest level Ka.

Conclusion

In conclusion the from the graphs and from the working out of the Keqi can state that the best conditions to process the haber process under is the lowest temperature that is usable because it increases the yield of the haber process in a linear regression which is a positive feedback increase in the yield of ammonia the optimized temperate was 200oC because it provided the highest yield. The other condition that was optimized during this experiment was pressure and after the experiment I found that the highest possible pressure is the optimum condition for this reaction to take place under. Because it gave the highest yield of ammonia compared to lower pressures which all provided lower yield.

Evaluation

The simulations that were used during this Essay were accurate enough to accept as possible theoretical yield but did not take into account of the possibility that some materials would be lost during the preparation for the haber process. It would have been better if I had more simulations and different type of simulations to check if the results I received from using these simulations were accurate or not and would increase the reliability of this experiment.

The limitations to using this method were the some simulations couldn't operate a catalyst which limited the amount of results I was able to obtain and didn't factor in any cost effectiveness into the reaction.

The haber process occurring in the presence of a catalysis does not affect the amount of NH3 that is produced by the reaction yet it only hastens the reaction by lowing the activation energy is takes for atoms to react. This would increase the rate of reaction without taking into consideration the geometric position that theses atoms need to react. A catalyst is a chemical that is used in a chemical reaction to speed up the rate of reaction with out the compound being used up in the reaction itself, meaning after the reaction the catalyst retains its structure and physical properties it had before the reaction took place. It works by lowering the activation energy of the reaction. The iron catalyst acts as a platform on which the Nitrogen and hydrogen atoms will bind on to before under going the reaction. The binding on to the catalyst is creates a transactional compound

N2(g)

nitrogen

+

3H2(g)

hydrogen

Fe

http://www. avogadro. co. uk/chemeqm/eqm_sign. gif

2NH3(g)

ammonia

Another Factor that I should have researched was the rate of reaction and possibly to the cost effectiveness of having a lower rate of reaction over the time effectiveness of having a high rate or reactions. Looking at the effect that the rate or reaction would have on at equilibrium

And working out possible ways to reduce the forward reaction to increase the yield of ammonia by adding a rate determining step for the forward reaction to encourage the forward reaction to reaction and produce ammonia but would discourage the backward reaction from according either by adding third party molecule such Sulphuric acid to create ammonium sulphate and can easily to separated by heating to 235oC because it sublimes to create ammonia and sulphuric acid and the gases are at different weights meaning using a gases filtration method and condense then separately. (NH4)2SO4(s) NH3(g) + H2SO4(g) http://image. tutorvista. com/content/equilibrium/reversible-reaction-equilibrium-state. gif

Another improvement would be to calculate the H of the reaction while looking at G and S of the reaction to allow to choose the most accurate best conditions for the reaction and most accurate cost effective option for the reaction. Because the having a positive H means the need more energy placed in which reduces the cost effectiveness of the reaction but may increase the yield of the ammonia while the G which measure reactions ability to reaction at room temperature which would increase the rate of reaction and the low temperature would mean the equilibrium would shift and allow the ammonia to be created in much more yield making the reaction cost effective and maximum conditions for the maximum yield. By working out the S and H I could use them to work out the amount of unused heat which is lost to the surroundings during the reaction, after this work out which reaction conditions provide the less heat lost to the surrounding while still providing an acceptable amount of yield. After working out the H, G and S if would help me make a more informed decision on which of the reaction conditions provided current industry yield and cost and work out which conditions provided either current industry yield at a lower cost or improved yield at a higher cost and ultimately work out which conditions produced greatest yield and at the lost possible cost.

Another improved for this experiment would be increasing the range of pressure that was used during the simulations because I noticed in the graphs that increasing the pressure post 1000 would make the production of ammonia not as effective as lower pressures are.