Increase of concentration of ethyl acetate

ASSIGN BUSTER

Firstly the aim of the experiment is to determine the yield, conversion and reaction rate by employing the principles of material balance with chemical reaction for batch reactions. The purpose of the experiment is to find out the factors affecting the rate of reaction to increases the conversion rate the yield of product produced. The hypothesis of the experiment is that the increase of concentration of Ethyl Acetate would also increase the rate of reaction. From two different concentrations of Ethyl Acetate (0. 01M and 0. 02M) have shown that the 0. 02M of Ethyl Acetate shows a increase in the rate of reaction and conversion rate of Sodium Hydroxide to Sodium Acetate.

Secondly the theory part shows the definitions of terms like saponification, batchwise reactions and factors that affect the rate of reaction. The most important definition is the saponification which is the hydrolysis of an ester under basic conditions to form an alcohol and the salt of a carboxylic acid.

Thirdly, the procedure section shows how to carry out the 3 major steps which are preparation of the reactant, the experimental setup and the procedures to carry out the experiment.

This is followed by the results and calculations which is about the calculation of the conversion percentage and yield of the reactions of different concentrations of Ethyl Acetate carried out in the experiment.

After the results and calculations, is the discussion part which discusses the results obtained, states some precautions to be taken while carrying out the experiment and the factors that affect the results.

Lastly the conclusion concludes the report by stating if the aim of the experiment had been reached and it also states that the hypothesis that the higher the concentration of the reactant, the faster the rate of reaction and conversion, has been proven.

REPORT ON MATERIAL BALANCE WITH CHEMICAL REACTION

1. Introduction

1. 1 Background Literature

Conversion of sodium hydroxide into sodium acetate is called saponification. It is the process of making soap. It is the reaction between an ester with a metallic base and water. It is also related to the process used to convert natural fats into soap. (Donohue 2009)

An alkali is a soluble salt of an alkali metal like sodium. It is used in soap-making whereby it was obtained from the ashes of plants. Now, the term alkali describes a base which neutralizes an acid. (Donohue 2009)

Alkalis used in soap making are sodium hydroxide (NaOH), also called caustic soda; and potassium hydroxide (KOH), also called caustic potash. (Donohue 2009)

Example: An example of the reaction is:

(Therese Lott’s Saponification Calculator – Standalone spreadsheet for calculating saponification values in handmade soapmaking.)

(http://www. freepatentsonline. com/6751527. html)

1. 2 Aim

The aim of this experiment is to determine the yield, conversion and reaction rate by employing the principles of material balance with chemical reaction for batch reactions. This will also enable us to find out factors to improve the yield and the rate of conversion and reaction.

1. 3 Hypothesis

The hypothesis of the experiment is that if the concentration is high, the yield together with the rate of conversion and reaction would also increase. Thus, from a 0. 02M concentration of Ethyl Acetate and 0. 01M concentration of Ethyl Acetate, the 0. 02M concentration would have a higher yield, rate of conversion and reaction. This is because at the start of the experiment the conductivity value was high but as the reaction precedes the conductivity value decreases showing the concentration and number of moles.

2. Theory

2. 1 Saponification

Saponification is the hydrolysis of an ester under basic conditions to form an alcohol and the salt of a carboxylic acid. Saponification is commonly used to refer to the reaction of a metallic alkali with a fat or oil to form soap. Saponifiable substances are those that can be converted into soap. In the experiment the desired product is sodium acetate. (Donohue 2009)

2. 2 Batchwise Reaction

A batchwise reaction is a reaction where by reactants are put in and the reaction is started. After the reaction has ended, the products are taken out and the equipment and all are washed to be prepared for the next experiment. Unlike steady state reaction it does not have a continuous input and output. (Singapore Polytechnic 2009)

2. 3 Percentage Conversion

Xa = moles of A reacted

Moles of A fed into the reactor x100%

It is defined as a fraction of reactants or feed that successfully reacted to form the desired product. The above formula calculates the amount of reacts converted into products. (Singapore Polytechnic 2009)

2. 4 Yield of A Product

YP = Moles of desired product formed

Moles of reactant fed into the reactor

Yield has 3 definitions. Firstly it is amount of desired product formed based on the amount of limiting reactants feed into the reaction. Secondly it is the amount of desired product obtained divided by the amount of reactant consumed. Lastly, it is also defined as the amount of product obtained divided by the theoretically amount of limiting reactant consumed. The above reaction calculates the amount yield based on just the limiting reactant. (Singapore Polytechnic 2009)

2. 5 Rate of Reaction

The rate of reaction is the amount of time taken for the chemicals to react totally. (Singapore Polytechnic 2009)

2. 6 Surface Area To Volume Ratio

The surface area to the volume ration affects the rate of reaction. The smaller the particle, the larger its exposed surface area. With a larger exposed surface area more particles can collide with one another causing more reactions to take place within a shorter amount of time. (Purchon 2006)

2. 7 Presence of a Catalyst

If a catalyst is involved in a reaction, the amount of energy needed to start the reaction (activation energy) decreases. Thus, the molecules in the reactions will gain more energy that is equal to or more than the activation energy. The higher amount of energy a molecules has, the more active it will become and more collisions will occur increasing the rate of reaction. However a catalyst is not involved in this experiment. (Purchon 2006)

2. 8 Pressure

Pressure is another factor that affects the rate of reaction. Pressure mainly affects gases. Gases can be compressed. Thus, as pressure increases, gaseous molecules are closely packed together which allows them to collide more frequently with one another. This is almost the same as changing the concentration as the number of molecules is increased within a specific area.

However the reaction is a liquid-liquid reaction so pressure does not affect the reaction in this experiment. (Purchon 2006)

2. 9 Concentration

Concentration affects the rate of reaction. The higher the concentration, the number of particles within a specific area increases. Thus, molecules are closely packed together and this increases the number of collisions between molecules so the rate of reaction increases. Concentration is similar to pressure where by the number of molecules in a specific area increases. (Purchon 2006)

2. 10 Temperature

Temperature also affects the rate of reaction. If the temperature is higher, the energy levels of the molecules increases and they would tend to more faster. Thus, this results in more effective collisions in a shorter amount of time. (Purchon 2006)

2. 11 Conductivity

Unlike Sodium Hydroxide, Ethyl acetate, Ethanol and Sodium acetate have negligible conductivity. Thus the conductivity value of the reaction is measured by the conductivity of Sodium Hydroxide. The conductivity is used to find the concentration of Sodium Hydroxide as the reaction proceeds. (Singapore Polytechnic 2009)

Fig. 1) Graph of conductivity values of Sodium Hydroxide against the concentration of Sodium Hydroxide.)

3. Procedure

3. 1 Preparation of chemicals

The MSDS of sodium hydroxide and ethyl acetate was read and the handling and disposal of the chemicals must be familiarized before the start of the experiment. Disposable gloves and chemical goggles were put on when preparing and handling the chemicals. 500 ml of 0. 01 M sodium hydroxide solution and 500 ml of ethyl acetate solution to the required concentration as discussed in Questions 1 and 2 of Pre-experiment Assessment was prepared. (CP4047 Lab Manual)

3. 1. 1 Preparing 500 ml of 0. 01 M sodium hydroxide solution:

The required volume of 0. 1 M NaOH stock solution was measured using a measuring cylinder and pour into the 500 ml volumetric flask. The solution in the volumetric flask was topped up with de-ionized water to the 500 ml-mark. A Stopper was placed on the flask, and it was shaken and inverted to mix the solution. (CP4047 Lab Manual)

3. 1. 2 To prepare 500 ml of ethyl acetate solution:

About 250 ml de-ionized water was poured into a 500 ml volumetric flask first. The required volume was measured using the micropipettor. The stock solution was dispensed into the 500 ml volumetric flask. The solution in the volumetric flask was topped up to the 500 ml-mark. A stopper was placed on

the flask, and was shaken and inverted to mix the solution. (CP4047 Lab Manual)

3. 2 Experimental setup

(CP4047 Lab Manual)

3. 3 Carrying out the Experiment

The prepared sodium hydroxide solution was poured into the reactor. The reaction conditions were adjusted to the predetermined levels (based on experimental methodology discussed with Lecturer). The reaction conditions were recorded, Eg. temperature, stirring speed, concentrations and volumes of reactants. Conductivity meter probe was positioned into the reacting mixture. The ethyl acetate solution was poured in and the timer was started immediately. The conductivity values (mS/cm) at a regular interval of 1 minute for 30 minutes of reaction time was recorded. After 30 minutes of reaction, the stirring device was stopped and the magnetic stir bar was removed from the mixture using the magnetic rod. The conductivity probe was also removed and rinsed thoroughly with de-ionised water. The reaction product mixture was poured into the plastic waste container. The glassware was rinsed and the experiment was repeated based on experimental methodology discussed with the Lecturer. At the end of the experiment, the conductivity probe was removed from the reacting mixture and rinsed thoroughly with de-ionised water. All chemicals were disposed in the plastic waste container and were brought to the waste together with any unused reactants to W314 for proper treatment and disposal. All the used glass-wares was rinsed and tidied up the work space. (CP4047 Lab Manual)

4. Results and Calculations

4. 1 Determining the Yield of Sodium Acetate at 15 Minutes

The yield of Sodium Acetate at 15minutes is determined with the concentration of Sodium Hydroxide as with the concentration, the number of mole of sodium hydroxide can be found out. Also, with the molar ratio of Sodium Hydroxide and Ethyl Acetate, the number of moles of Ethyl Acetate can be determined. With the use of the yield formula, the yield of Ethyl Acetate can be calculated.

4. 2 Yield When 0. 01M of Ethyl Acetate Used

5. Discussion

5. 1 Factors Affecting Rate of Reaction

Firstly the concentrations of Ethyl Acetate used were 0. 01M and 0. 02M which means that for 0. 01M of Ethyl Acetate was obtained by diluting 0. 49cm3 of pure Ethyl Acetate and 0. 02M was obtained by diluting 0. 92cm3 of pure Ethyl Acetate. By comparing the graphs (Fig 3 and 4) above, the reaction (0. 02M) was the fastest. This was due to the concentration factor. The higher the concentration, the faster the rate of reaction as the increase in concentration means that there are more molecules in a specific area.

Other factor like temperature and pressure were keep at a constant (standard room conditions). There was no catalyst involved the experiment. Thus, these other factors did not affect the rate of reaction.

5. 2 Factors Affecting Conversion and Yield

The conversion of Sodium Hydroxide and the yield of Sodium Acetate will never be a 100% due to the technical equipment and unforced human errors. It is also due to constrains in the lab like equipment or the duration of the experiment. The longer the reaction, more conversion and yield could have been produced.

5. 3 Factors Affecting the Conductivity Values

The concentration of Sodium Hydroxide affects the conductivity value of the reaction. If the concentration of Sodium Hydroxide is high, the conductivity value will also be high. Thus, as the reaction proceeds, the conductivity drops as the concentration of the Sodium Hydroxide decreases as it is being reacted away. For the 0. 01M reaction, Fig 4. 2. 2 show that the concentration decreases significantly. However, for the 0. 02M reaction, Fig 4. 3. 2 shows some fluctuations in the drop of the concentration of Sodium Hydroxide. This could be because of the equipment. The equipment, the conductivity probe and the machine has been known to turn off randomly during the reaction. Thus there was some irregularities in the drop of concentration for the 0. 02M reaction.

5. 4 Precautions to Be Taken

During the experiment the Ethyl Acetate should always be handled in the fume hood as it would decompose in the open, thus affecting the concentration of the Ethyl Acetate and to prevent it from spilling anywhere else in the laboratory. Gloves should also be worn to prevent bacteria from contaminating the reaction or chemicals and to also protect our hands from

the chemicals. Goggles should also be worn to protect our eyes from chemicals splashing into our eyes.

5. 5 Comparison of conversion and yields of different concentration of Ethyl Acetate

The yield of the reaction of 0. 01M Ethyl Acetate is 0. 62 while the yield of the reaction of 0. 02M Ethyl Acetate is 0. 76. The second reaction of 0. 02M has a higher yield due to the higher concentration of Ethyl Acetate. This is because the concentration of the reactants is more due to the increase in concentration of Sodium Hydroxide thus, producing more products whereby the yield of Sodium Acetate increases. However both the experiments did not produce a 100% yield because of human error and constrains of technical equipment. Even if a catalyst was added, the yield will be the same as the catalyst will only increase the rate of reaction and affect the yield.

6. Conclusion

In conclusion, the higher the concentration of Ethyl Acetate used, the faster the rate of reaction together with a higher conversion percentage of Sodium Hydroxide. The concentration of Sodium Hydroxide affects the conductivity values of the reaction because the results show that the conductivity decreases as the reaction proceeds because the concentration of Sodium Hydroxide also decreases as the Sodium Hydroxide was being reacted away. Therefore, the hypothesis is proven to be true.

The aim of the experiment was met as results state that with a higher concentration of Ethyl Acetate, the rate of reaction together with the rate of conversion increases. The concentration of the Ethyl Acetate reacting with

Sodium Hydroxide in a reactor as time passes by was studied. However the experiment could be improved by adding in a catalyst or increasing the temperature to increase the rate of reaction and conversion rate.