Investigating the effect of different concentrations of concentrated sulfuric acid (%)on the rate of reaction, and the Turnover Number in the esterification of ethanoic acid and ethanol

Word count: 2990

Research question

What is the effect of varying concentration (0.10%, 0.15%, 0.20%, 0.25%, and 0.30%) of concentrated sulfuric acid with respect to ethanoic acid(%), on the rate of reaction($mol\,L^{-1}s^{-1}$) and the turnover number(s^{-1}) in the esterification of ethanoic acid and ethanol, while keeping the reactants volume constant and temperature of the system?

Introduction

Esterification is a reaction that involves a Carboxylic acid and an Alcohol to form a substance known as an Ester. A complex chemical reaction occurs between the carboxyl and hydroxyl functional group in the presence of an acid catalyst to form an ester linkage with a water molecule removed as a byproduct. For example, when Ethanol is treated with ethanoic acid in the presence of sulfuric acid to form an ester known as Ethyl acetate. Esters are organic compounds with a sweet pleasant smell with comparatively lower boiling points and can be found naturally or synthesized artificially . This investigations explores that synthesis of the ester Ethyl ethanoate or Ethyl Acetate, which is primarily used as coating solvent for paints, varnishes, process solvent in the pharmaceutical industry, it is also used for manufacturing of artificial leather and lastly it is also used in certain household products such as nail polish remover and artificial sweetener[1].

In esterification, the condensation reaction between a carboxylic acid and alcohol is significantly slower because it requires high activation energy for the nucleophilic attack by the alcohol on the carbonyl carbon. A homogeneous catalyst like sulfuric acid is added to the process, providing an alternative reaction pathway with a significantly lower reaction activation energy. A homogeneous catalyst is a catalyst which is in the same state as the reactants in the chemical reaction, which results in an increase in the rate of reaction as the reactants and catalyst are in the same state. Moreover, by lowering the activation energy, catalysts can exponentially increase the rate of esterification by allowing the reaction to reach an equilibrium point significantly faster with higher yields of products. However, as the rate of reaction is directly proportional to the

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Wexler, P. (2014). *Encyclopedia of toxicology* (Vol. 3). Amsterdam: Academic Press. Retrieved from https://www.sciencedirect.com/referencework/9780123864550/encyclopedia-of-toxicology concentration of sulfuric acid, as sulfuric acid concentration increases the rate of successful collisions between reactant molecules increases, resulting in a faster rate of product formation. Catalysts are one of the most important aspects in chemical and pharmaceutical industries, they can provide more yield in a cost effective manner. I personally got interested in esterification because of my uncle, as he owns a pharmaceutical company that manufactures the paint (ester) that is used for coating medicines. When I visited the manufacturing plant once, he explained to me that it is crucial to use the correct ratio or amount in a reaction to maximize the yield of a product, which additionally is efficient and cost effective at the same time.

Background Information

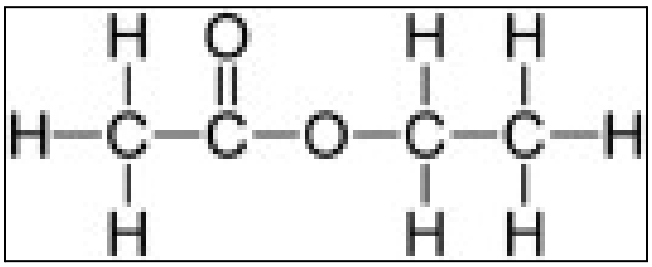

Figure 1. Structural Formula of ethyl ethanoate **(Wexler, vol. 3)**

The esterification of ethanol and ethanoic acid forms the ester, ethyl ethanoate or also known as ethyl acetate. Esters have the functional group (R-COO-R). Esters are the product of condensation of carboxylic acid and alcohol. In ethyl ethanoate, the carboxyl group comes from ethanoic acid and hydroxyl group comes from ethanol and they are combined to form water as a byproduction.

Chemical Reactions and Equations

$$CH_3COOH_{(aq)} + CH_3CH_2OH_{(aq)} - H_2SO_4 \rightarrow CH_3COOH_2CH_{3(aq)} + H_2O_{(aq)}$$ **Equation 1**

Equation 1 shows the reaction and conversion of ethanoic acid and ethanol in presence of sulfuric acid as a catalyst, to form ethyl ethanoate and water as products. Sulfuric acid as a catalyst is added to increase the rate of reaction, but excessively high concentration can cause side reactions and affect the yield of the product. **Hence it is crucial to use controlled or calculated ratios catalyst (sulfuric acid) for ensuring an optimal rate of reaction without minimum side reactions.**

Reaction that includes esterification consists of five steps mechanisms :

1. Carbocation or cation formation
2. Delocalization of the carbocation

3. Transfer of proton
4. Formation of the pi bond
5. Formation of Ester

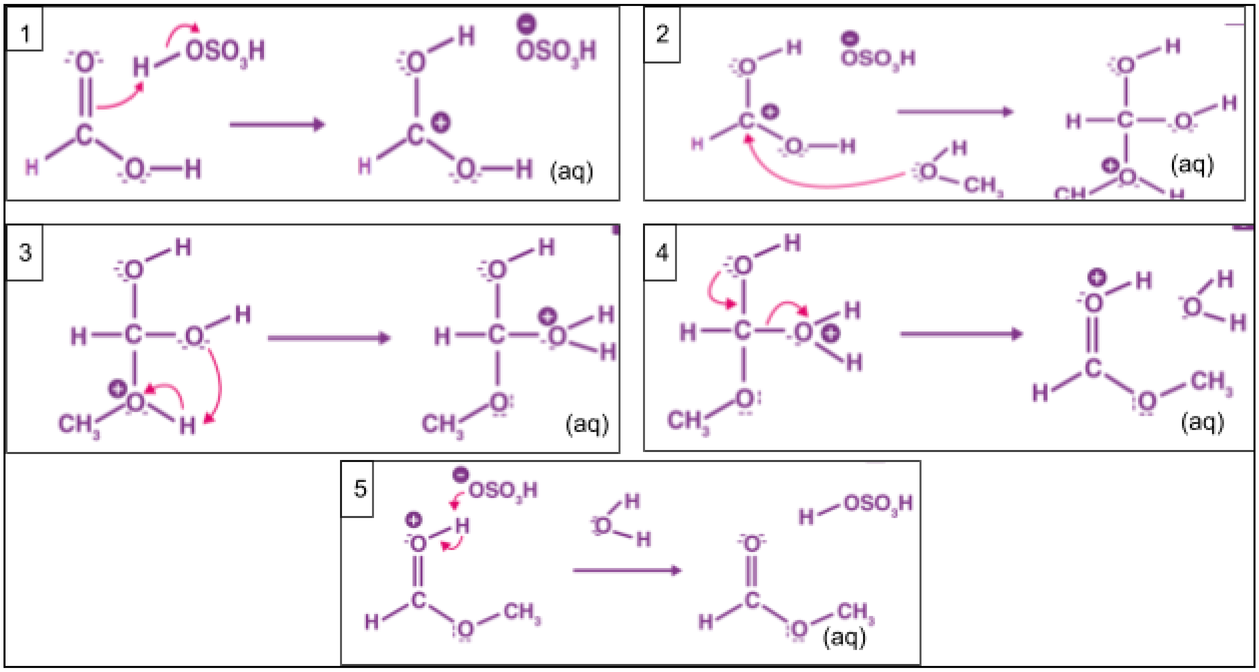

Figure 2. Five Step mechanisms of esterifications[2].

Turnover Number

The turnover number is the maximum number of molecules of reactant that can be converted into product per catalytic molecule of a given concentration of catalytic per unit time.

$$k_{cat} = \frac{V_{max}}{[E_t]} \qquad \textbf{Equation 2}$$

Where $\mathbf{K_{cat}}$ is the turnover number, $\mathbf{V_{max}}$ is the maximum reaction rate ($mol\ L^{-1} s^{-1}$)and ***[E_t]*** is the moles of the catalyst(mol)[3] **(Chemistry LibreTexts).** It represents the total number of reaction cycles a single catalytic site of a catalyst can perform.

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[2]**BYJU'S. (2022). Esterification (Alcohol & Carboxylic acid) - Reactions Mechanism & Uses with Videos. Retrieved July 24, 2024, from BYJU'S website: https://byjus.com/chemistry/esterification/**

[3] Chemistry LibreTexts. (2013, October 2). Turnover Number. Retrieved July 25, 2024, from Chemistry LibreTexts website: https://chem.libretexts.org/Bookshelves/Biological_Chemistry/Supplemental_Modules_(Biological_Chemistry)/Enzymes/Enzymatic_Kinetics/Turnover_Number

Hypothesis

Increasing the concentration of sulfuric acid (%) with respect to ethanoic acid, while keeping the temperature (100°C), pressure(1 atmospheric pressure) and volume of reactants constant(106 grams) throughout the experiment, will result in an increase in the rate of reaction with a positive linear relationship between the catalyst concentration ,and the rate of the reaction. While the turnover number for sulfuric acid as a catalyst will also increase with increasing concentrations of the catalyst.

Independent variable

Different concentrations(%) of concentrated sulfuric acid (**0.10%, 0.15%, 0.20%, 0.25%**, and **0.30%** with respect to ethanoic acid) used in the esterification of ethanoic acid and ethanol.

Dependent variable

The rate of reaction ($mol\,L^{-1}s^{-1}$**)** and the turnover number, determined by the change in acid value ($mg\ KOH/gram$) of the reaction mixture over the period of one hour. The acid value is measured by the volume of 0.26 normal NaOH required to titrate the sample of the reaction mixture solution (0.1 **gram**) and to identify the endpoint of titration, that is when the color of the reaction mixture solution changes from orange to blue.

Controlled variables

Controlled variable	Purpose of control	Method for control
volume of ethanoic acid	Varying volumes of reactants will not give reliable results and may hinder the rate of esterification. Hence ethanoic acid is the limiting reactant only a certain volume of it needs to be used for each experiment.	Using an electronic weighing balance, to measure 60 grams of powdered ethanoic acid for each experiment.
volume of Ethanol	Varying volumes of reactants will not give reliable results and may hinder the rate of esterification. Hence Ethanol is used in excess quantity for the experiment,	Using an electronic weighing balance, to measure 46 grams of Ethanol for each experiment.
Temperature	Using different temperatures or uncontrolled temperatures can hinder and affect the rate of esterification.	By running the reaction in a temperature-controlled environment, using a heating plate or water bath specific temperature ($100 \pm 2°C$), while monitoring and maintaining the temperature throughout the experiment using a thermometer.
Pressure	varying pressure can hinder and affect the rate of esterification.	By performing the reaction at 1 atmosphere pressure.
Reaction time	The reaction rate or rate of esterification is measured overtime and choosing a consistent time is crucial as it allows accurate and direct comparison between the experiments.	Setting a specific time to measure the rate of esterification i.e by obtaining the Acid value and the time will be (1 hour). This can be ensured using a timer in order to maintain the same time duration for all reactions.
Normality of standard solution of Sodium Hydroxide ($NaOH$)	If the Normality of the standard solution varies, it will affect the acid value.	Verify the Normality of $NaOH$ solution by standardizing it with KHP.

Table 1. Controlled variables

Apparatus and materials required

Sr.no	Apparatus	Quantity	Uncertainty
1	beaker 200mL	x3	±0.1 cm3
2	conical flask 250mL	x1	±1.0 cm3
3	round Bottom flask	x2	-
4	volumetric flask	x1	±0.30
5	graduated glass pipette 0.1 mL	x2	±0.001 mL
7	glass stirring rod	x1	-
8	thermometer	x1	±1 C
9	glass funnel	x1	-
10	burette 25mL	x1	±0.05 mL
11	burette stand	x1	-
12	condenser	x1	-
13	electronic weighing balance	x1	±0.01 gram
14	Hot Plate	x1	-
15	latex non powder hand gloves	x10 pairs	-
16	safety goggles	x2 pairs	-
17	spray bottle	x1	-
18	Boiling chips	x12 chips	-
19	pipette bulb	x2	-
20	burette clamps	x3	-
21	spatula	x1	-

Table 2. Lists of apparatus and materials required

Chemicals required

Sr.no	Chemical	Chemical formula	Quantity
1	Glacial ethanoic acid		1000 mL
2	Ethanol	C_2H_6O	1200 mL
3	Concentrate sulfuric Acid	H_2SO_4	50 mL
4	Potassium hydrogen phthalate	$C_8H_5KO_4$	2 grams
5	Sodium hydroxide pellets	NaOH	15 grams
6	distilled water	H_2O	500mL
7	Bromothyml blue indicator	$C_{27}H_{28}Br_2O_5S$	125mL

Table 3. List of chemicals required

Methodology and procedure

Methodology for preparing standard solution for 0.26 molar sodium hydroxide (NaOH) :

1. Using an electronic balance weigh 1 gram of sodium hydroxide (NaOH) pellets in a clean and dry beaker.
2. Then add a small volume of distilled water into the beaker, and thoroughly stir it with a glass rod until the pellets completely dissolve.
3. Transfer the solution to a 250 mL volumetric flask using a glass funnel.
4. Moving on, the beaker, glass rod and glass funnel needs to be rinsed at least three times with distilled water, while each time adding the same water into the volumetric flask to ensure that the solute is completely transferred.
5. The distilled water should only be added to the volumetric flask until its level reaches the graduation mark.
6. Place a stopper on the top of the volumetric flask and turn it over for at least 5 to 10 times, to ensure the solution is mixed thoroughly.
7. The 0.5 molar sodium hydroxide (NaOH) solution is then kept overnight in the volumetric flask itself, prior to any use[4]

[4] Bylikin, S., Horner, G., Grant, E. J., & Tarcy, D. (2023). *Oxford Resources for IB DP Chemistry: Course Book* (2023 EDITION). Oxford University Press. (Original work published 2023)

Methodology for preparing the reactants in (1:1 reaction ratio):

- 60 grams of ethanoic acid is to be weighed in a beaker on an electronic balance.
- 46 grams or of Ethanol is to be measured using the electronic balance.
- Transfer both 60 grams of ethanoic acid ,and 46 grams of Ethanol directly into a 250 mL round bottom flask.
- Hence, after transferring the reactants thoroughly mix them by either using the neck of the round bottom flask or using a glass rod.
- Add 5 to 6 boiling chips into the reaction mixture for evenly distributing heat throughout the reaction mixture.

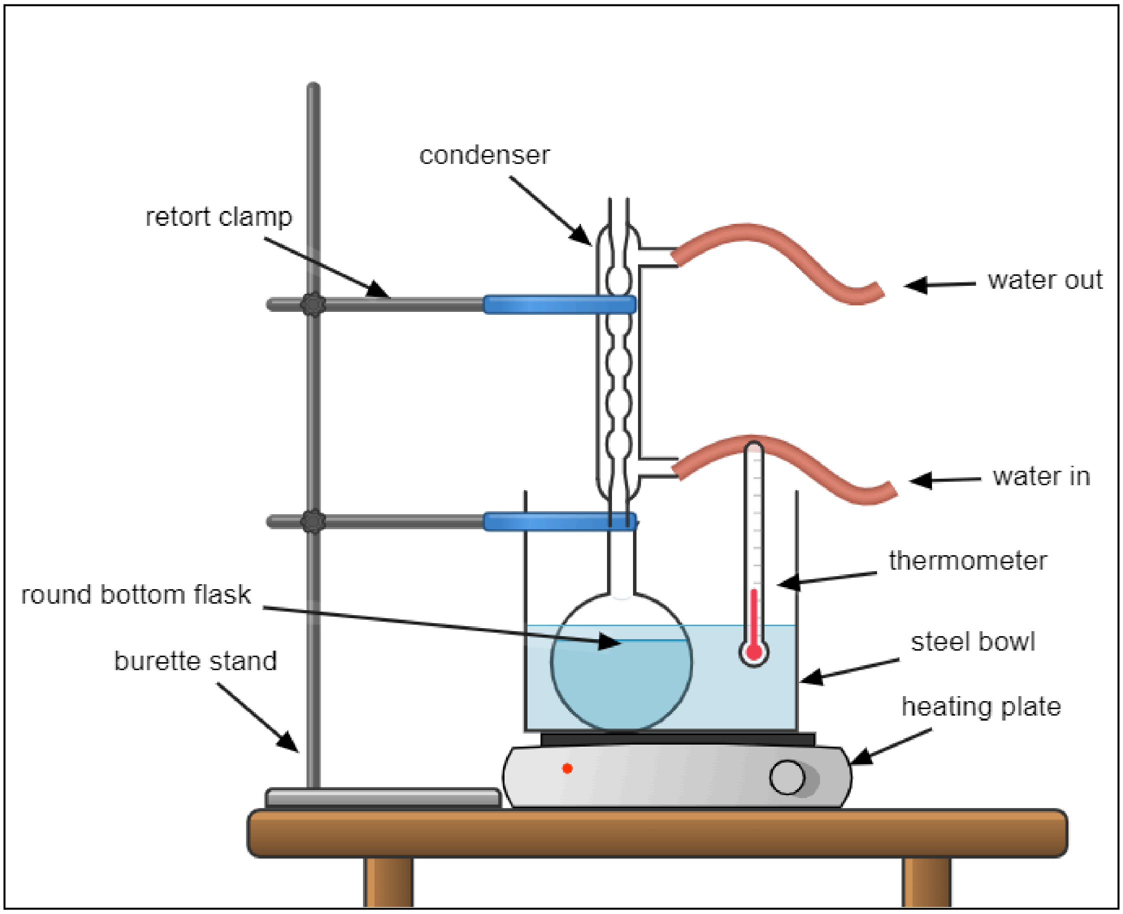


Figure 2. Illustrated setup for the experiment. Made with chemix[5]

[5] Chemix. (2019). Chemix - Draw Lab Diagrams. Simply. Retrieved August 16, 2024, from Chemix.org website: https://chemix.org

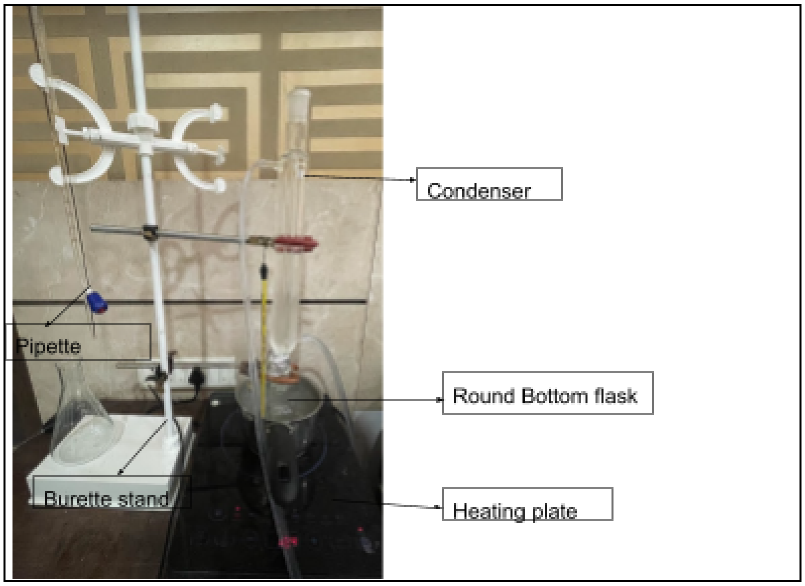


Figure 3. Actual setup for the experiment

Methodology for measuring the acid value after the reaction

- Take 50 mL of ethanol in a conical flask and neutralize it with 0.26 N sodium hydroxide.
- Transfer a accurately measured quantity 0.1 gram of reaction mixture into the conical flask and stir it well.
- Add 2 drops of **Bromothymol blue** into the conical flask.
- Then titrate it with 0.26 N and standardize the sodium hydroxide unit the solution in the conical flask turns from **yellow to blue** and measure the burette reading.

Risk Assessment

Safety concerns

Chemical	Formula	Potential Risks	Precautions
Sulfuric Acid	H_2SO_4	Highly corrosive and can cause severe burns to skin, eyes, respiratory system	Always wear PPE: gloves, goggles, mask. Use the pipette carefully; wash thoroughly after use.
Sodium Hydroxide	NaOH	Corrosive base and causes irritation and burns to skin, eyes, respiratory issues	Always wear PPE: gloves, goggles, mask. Add water carefully to avoid heat release; store in a dry place.
Potassium Hydrogen Phthalate (KHP)	KHP	May irritate skin, eyes, respiratory system if inhaled[6]	Always wear PPE kit, gloves, goggles, mask when handling.

Table 4. Safety concerns

Environmental considerations

Environmental considerations consist of proper disposal of the reaction mixture and sodium hydroxide. Once the experiment is completed and readings are measured. Place the ethyl ethanoate in a designated waste container and handing it over to the lab technicians, where they will neutralise and dispose of it accordingly with respect to local or state regulations.[6]

Sodium hydroxide (**NaOH**) is harmful to aquatic environments if not disposed of responsibly. To dispose of the sodium hydroxide solution made, firstly neutralise it with an acid strong acid such hydrochloric acid or sulfuric acid and dispose it into a designated waste container and handed it over to lab technician for further disposal with respect to local or state regulations [7]

Ethical considerations

There were no ethical considerations in this experiment because the methodology did not involve any living organisms and disposal of chemicals was done by following proper methodology and local regulation to ensure no harm is caused to the environment.

[6] Solutions, N. C. (2015, December 8). 404 - Uh oh, I think we lost chemistry - Parchem Fine & Specialty Chemicals. Retrieved from www.parchem.com website: https://www.parchem.com/siteimages/Attachment/GHS%20Ethyl%20Acetate%20MSDS.pdf

[7] New Jersey Department of Health. (2015). *Right to Know Hazardous Substance Fact Sheet Description and Use Hazard Summary Reasons for Citation*. Retrieved from https://nj.gov/health/eoh/rtkweb/documents/fs/1706.pdf

Raw Data Collection
Quantitative Data

Concentrations of H_2SO_4 w.r.t ethanoic acid in %	Acid value of reactants (without catalyst) mg KOH /g	Acid value of reactants (with catalyst) mg KOH /g	ΔAcid value (change in Acid value) mg KOH /g
0.0	466.75	Not Applicable	Not Applicable
0.1	495.92	510.51	14.59
0.15	452.16	466.75	14.59
0.20	452.16	481.33	29.17
0.25	452.16	525.09	72.93
0.30	452.16	554.268	102.108

Table 5. Initial acid values for reaction mixture

Concentrations of H_2SO_4w.r.t ethanoic acid in %	Trials			Average Acid value mg KOH /g
	Acid value Trial 1 mg KOH /gram	Acid value Trial 2 mg KOH /gram	Acid value Trial 3 mg KOH /gram	
0.0	452.16	437.58	451.2	446.98
0.10	277.13	262.54	254.69	264.78
0.15	218.71	204.20	200.76	207.89
0.20	189.62	175.03	172.79	179.14
0.25	131.27	116.69	115.56	121.17
0.30	87.51	72.92	72.92	77.78

Table 5. Final acid values after 1 hour

Data Processing

Calculation for preparing and standardizing NaOH

Calculation of concentration of sulfuric acid with respect to ethanoic acid (in mL)

$$\frac{x\%\ of\ H2SO4}{100} \times Given\ weight\ =\ weight\ of\ H2SO4$$

$$\frac{0.10\%}{100} \times 60\ grams\ =\ 0.06\ grams$$

Density of sulfuric acid = $1.8\ gram/cm^3$

$$\frac{Mass}{Density} = Volume$$

$$\frac{0.06}{1.8}\ =\ 0.03\ mL$$

Calculation for Acid Value for 0.10% concentration

$$ACID\ VALUE\ (mg\ KOH\ /gram)\ =\frac{Burette\ reading \times 56.1 \times Molarity\ of\ standard\ solution}{Sample\ weight}$$

$$ACID\ VALUE\ for\ 0.10\%\ H2SO4\ w.r.t\ ethanoic\ acid\ =\ \frac{2 \times 56.1 \times 0.26}{0.1}$$

$$=\ 291.72\ mg\ KOH\ /gram$$

$$Final\ ACID\ VALUE\ (mg\ KOH\ /gram)\ =\ ACID\ VALUE\ -\ Change\ in\ Acid\ value\ due\ to\ H2SO4$$

Note* The Acid value for the reaction mixture was measured before and after the addition of sulfuric acid (catalyst) such that we measure the Acid value exclusively for ethanoic acid.

$$Final\ ACID\ VALUE\ =\ 291.72\ -\ 14.59$$

$$Final\ ACID\ VALUE\ =\ 277.13\ mg\ KOH\ /gram$$

Calculating initial and final concentrations of ethanoic acid

Calculation rate of reaction for 0.10% concentration

$$Rate\ of\ esterification(\ mol\ L^{-1}s^{-1}) = \frac{Initial\ moles\ of\ ethanoic\ acid - final\ moles\ of\ ethanoic\ acid}{3600\ seconds}$$

$$= \frac{1-0.53}{3600} = 1.29\ \times\ 10^{-4}\ mol\ L^{-1}s^{-1}$$

Calculation concentration of Sulfuric acid for 0.10% concentration

$$Mass\ of\ sulfuric\ acid\ (gram)$$

$$= Percentage\ of\ H2SO4\ w.r.t\ ethanoic\ acid\ \times\ mass\ of\ ethanoic\ acid(g)$$

$$= \frac{0.10}{100} \times\ 60\ = 0.06\ gram$$

$$Moles\ sulfuric\ acid\ (mol) = \frac{given\ weight}{molar\ mass}$$

$$= \frac{0.06}{98.079}\ = 6.11\ \times\ 10^{-4} mol$$

$$Volume\ of\ sulfuric\ acid\ (mL) = \frac{mass\ of\ sulfuric\ acid}{density\ of\ sulfuric}$$

$$= \frac{0.06}{1.83}\ =\ 0.03\ mL$$

Turnover number for 0.10% concentration

$$Turnover\ number\ (s^{-1}\ )\ = k_{cat} = \frac{V_{max}}{[E_t]} = \frac{Rate\ of\ reaction}{moles\ of\ catalyst}$$

$$= \frac{1.29\times10^{-4}}{6.11\times10^{-4}}\ =\ 0.211\ s^{-1}$$

Calculating Uncertainty and error propagation

Note* The overall percentage uncertainty will be slightly higher because of using a very small volume of reaction mixture (0.1 mL) for analysis in this experiment.

1. Percentage uncertainty with respect to the molarity of NaOH solution:

Uncertainty in weighing of NaOH

$$uncertainty\ (\%) = \frac{uncertainty}{measurement} \times 100$$

$$uncertainty\ (\%) = \frac{0.01\ gram}{0.5\ gram} \times 100$$

$$uncertainty\ (\%) = 2\%$$

Uncertainty of 0.26 Molar NaOH solution in volumetric flask

$$uncertainty(\%) = \frac{0.30\ mL}{250\ mL} \times 100$$

$$uncertainty\ (\%) = 0.12\%$$

2.Percentage uncertainty of standardizing the 0.26 Molar NaOH solution with KHP

Uncertainty in weighing of KHP

$$uncertainty\ (\%) = \frac{0.01\ gram}{0.580\ gram} \times 100$$

$$uncertainty\ (\%) = 1.7\%$$

Uncertainty of standardizing 0.26 Molar NaOH solution with KHP

$$uncertainty\ (\%) = \frac{0.1\ mL}{10.9\ mL} \times 100$$

$$uncertainty\ (\%) = 0.91\%$$

3.Percentage uncertainty for the preparation of the reactants (weighing scale and H_2SO_4 pipette)
Weight of ethanoic acid and ethanol

$$uncertainty\ (\%)\ ethanoic\ acid\ =\ \frac{0.01\ gram}{60\ gram} \times\ 100$$
$$uncertainty\ (\%)\ ethanoic\ acid\ =\ 0.01\%$$

$$uncertainty\ (\%)\ Ethanol\ =\ \frac{0.01\ gram}{46\ gram} \times\ 100$$
$$uncertainty\ (\%)\ Ethanol\ =\ 0.02\%$$

Volume of sulfuric acid used in the experiment

$$uncertainty\ (\%)\ Sulfuric\ acid\ =\ \frac{0.001\ mL}{0.03\ mL} \times\ 100$$
$$uncertainty\ (\%)\ Sulfuric\ acid\ =\ 3.33\%$$

H_2SO_4 concentration (%)	H_2SO_4 concentration in (mL)	Uncertainty(%)
0%	Not applicable	Not applicable (0)
0.10%	0.03 mL	3.3%
0.15%	0.05 mL	2.0%
0.20%	0.06 mL	1.6%
0.25%	0.08mL	1.2%
0.30%	0.09 mL	1.1%

Table 6. Total (%) uncertainties during preparation of reactant

4. Measuring the Acid value (burette, pipette)

$$uncertainty\ (\%)\ Initial\ Acid\ value\ with\ catalyst\ with\ pipette\ =\ \frac{0.001\ mL}{0.1\ mL} \times\ 100$$
$$uncertainty\ (\%)\ Initial\ Acid\ value\ with\ catalyst\ with\ pipette\ =\ 1\%$$
$$uncertainty\ (\%)\ Initial\ Acid\ value\ with\ catalyst\ with\ burette\ =\ \frac{0.05\ mL}{3.0\ mL} \times\ 100$$
$$uncertainty\ (\%)\ Initial\ Acid\ value\ with\ catalyst\ with\ burette\ =\ 3.3\%$$

Concentration (%)	**Average Acid value after adding catalyst**	**Uncertainty of pipette** (%)	**Uncertainty of burette** (%)	**Total uncertainty of acid value (before reaction)**(%)
0%	Not applicable	1%	Not Applicable	Not Applicable
0.10%	510.51	1%	1.42%	2.42%
0.15%	466.75	1%	1.56%	2.56%
0.20%	481.33	1%	1.5%	2.5%
0.25%	525.09	1%	1.35%	2.35%
0.30%	554.268	1%	1.31%	2.31%

Table 7. Total (%) uncertainties for acid value before the reaction

Concentration (%)	**Acid value after one hour**	**Uncertainty of pipette** (%)	**Uncertainty of burette** (%)	**Total uncertainty of acid value (after reaction)**(%)
0%	446.98	1%	1.65%	2.65%
0.10%	264.78	1%	2.75%	3.75%
0.15%	207.89	1%	3.57%	4.57%
0.20%	179.14	1%	4.16%	5.16%
0.25%	121.17	1%	6.25%	7.25%
0.30%	77.78	1%	10%	11%

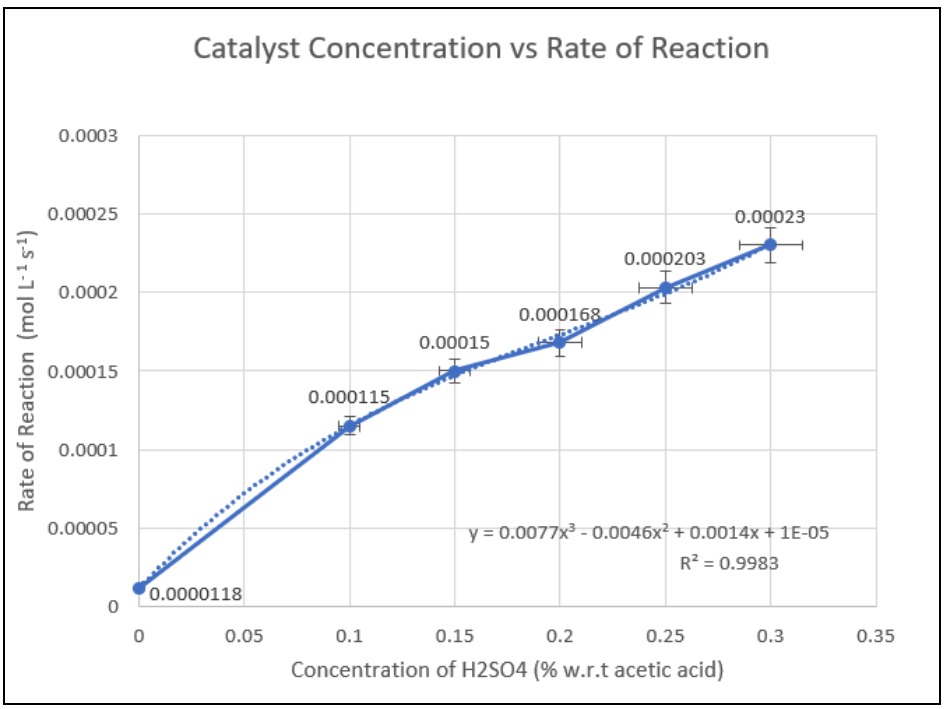
Table 8. Total (%) uncertainties for acid value after the reaction

Processed Data

Concentration (%)	**Turnover number** (s^{-1})	**Rate of Reaction** ($mol\ L^{-1}s^{-1}$)	**Total uncertainty** (%)
0	Not Applicable	1.18×10^{-5}	9.06 %
0.10	0.211	1.29×10^{-4}	14.23 %
0.15	0.163	1.50×10^{-4}	13.07 %
0.20	0.137	1.68×10^{-4}	14.02 %;
0.25	0.137	2.03×10^{-4}	15.56 %
0.30	0.125	2.30×10^{-4}	19.17 %

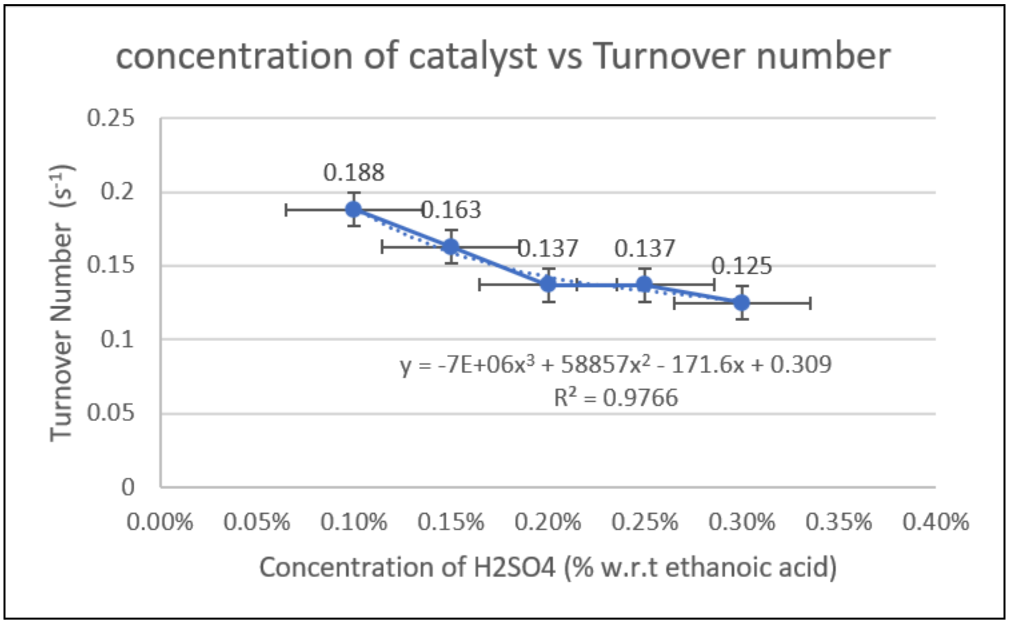
Table 9. Final processed data table with uncertainties

Data analysis



Graph 1. Concentration of catalyst vs rate of reaction

The above graph represents the relationship between the concentration of sulfuric acid (catalyst) and the rate of reaction in the esterification of ethanoic acid and ethanol at 100 C. In **Graph 1** there is a non-linear relationship between the two variables as it can be clearly seen that rate of reaction does not increase with the concentrations in a linear manner.



Graph 2. Turnover number of (Sulfuric acid)

The above graph represents the relationship between the concentrations of sulfuric acid (with respect to ethanoic acid) and the Catalytic efficiency. In **Graph 2** it is clearly evident that the catalytic efficiency of sulfuric acid decreases with increasing concentrations.

Conclusion

The research question for the experiment was to investigate the effect of varying concentrations (%)of concentrated sulfuric acid (0.10%, 0.15%, 0.20%, 0.25%, and 0.30% with respect to ethanoic acid) as an catalyst in the esterification of ethanoic acid and ethanol on the rate of reaction and the catalytic efficiency of sulfuric acid. The results obtained from the experiment clearly represent that the rate of reaction does increase as the concentration of the catalyst increases. As evident in **Graph 1,** that adding a catalyst significantly increases the rate of reaction as at 0% catalyst concentration the rate of reaction is is just $1.18 \times 10^{-5} mol^{-s}$,but at 0.10% concentration the rate of reaction is $1.29 \times 10^{-4} mol^{-s}$, where the rate increased **10** times than that at 0% concentration. However after the concentration of 0.10% the increase in rate of reaction for the successive concentrations are 0.10% to 0.15% is **1.16** times, 0.15% to 0.20% is **1.12** times , 0.20% to 0.25% is **1.21** times and 0.25% to 0.30% is **1.13** times. Additionally the **R^2** obtained by fitting the data into a third-degree polynomial model consists of the value of **0.9968**, indicating a strong correlation between the concentration of the catalyst and the rate of reaction.

Moving on, to the turnover number of sulfuric acid in the esterification of ethanoic acid and ethanol, it was observed that as the concentration of catalyst increases the values of turnover number decreases across the successive concentrations. Evident in **Graph 2** that the values of turnover number instantly decreases after **0.10%** concentration, however the turnover number for 0.20% and 0.25% concentration is the same suggesting that the catalyst's efficiency diminishes with higher concentration. The decrease in the turnover number can be explained because of reasons such as, Inhibition of catalyst by water. As esterification is an equilibrium (reversible) reaction, and with higher catalyst concentrations the protonation of water molecules happens, which can potentially increase the reverse hydrolysis reaction and eventually reduce the turnover number for successive sulfuric acid concentration.Additionally one of the major factor that can be concluded from the experiment is that despite increasing the amount of catalysts reacting molecules are in equal quantities for all successive concentrations, which reduces the turnover number. Hence the optimal amount of catalyst to be used depends on the quantity of reactants. Therefore, increasing the concentrations of the catalyst still increases the rate of reaction but not the efficiency of the catalyst in this particular esterification of ethanoic acid and ethanol.[8]

Evaluation

Strengths of the experiment

The experiment consisted of a well focused research question that is specifically addressing the effects of increasing concentration of catalyst on the rate of reaction and the turnover number of the catalyst. Firstly, following the methodology for this experiment I was able to control other external factors that affect the rate of reaction such as temperature, maintained at 100±2°C, then keeping the concentration of reactant constant and performing the experiment at 1 atmosphere pressure. Additionally using precise apparatus such as the pipettes, burettes and electronic weighing balance that would have minimized the margins of errors and uncertainty. Lastly, partially rejecting the my hypothesis statement that hypothesised that there would be a linear relationship between concentration of catalyst, and rate of reaction and the turnover number.

[8] Kaplan. (2020). Step by Step Solution. Retrieved December 4, 2024, from Vaia website: https://www.vaia.com/en-us/textbooks/chemistry/mcat-general-chemistry-review-2020-2021-2021-edition/chapter-5/problem-6-what-would-increasing-the-concentration-of-reactan/

Limitation and weakness of the experiment

Limitation - weakness	Impact on the results	Potential solutions
Small volume of the reaction mixture analyte, (0.1 gram)	Analysis of small volumes increases the impact of instrument precision errors leading to higher uncertainty or errors.	Using larger volumes of the reaction mixture analyte in order to reduce measurement errors and uncertainties.
Only 3 trials done per each concentration treatments because of resource limitation and potential safety concerns	A Smaller number of trials potentially consists of risks of random errors that could impact the results significantly.	Conducting more trials (at least 5) with sufficient resources and improved safety measures.
Higher uncertainties (%)	The values of uncertainties(%) range from 9.06% to 19.17%, which means the uncertainties may have affected the results of the experiment.	As mentioned earlier, using larger volumes of analyte, with more precise equipment and an enhanced methodology.

Table 10. Limitation-weakness of the experiment with its impact on the results and potential solutions

Improvements and further investigations

An extension for this experiment could be to investigate the efficiency and rate of reaction of different heterogeneous catalysts in the esterification reaction such as Aluminium Oxide (**Al2O3)** and Iron Oxide (**Fe2O3**) as heterogeneous catalysts. Despite homogeneous catalysts such as sulfuric acid and hydrochloric acid rapidly increasing the rate of esterification reaction, they cause acidic wastes, side reactions, and corrosion, and importantly they cannot be reused as they cannot be separated from the reaction mixture after the product formation.[9]

Additionally, Investigating the effect of Sulfuric acid (**H_2SO_4**) as catalyst on the rate of reaction in other types of esterification reactions that involves different reactants such as Methanoic acid with Methanol, Propanoic acid with Butanol, and Citric acid with Glycerol. Lastly, modeling the rate of esterification reactions that do not consist of fixed amounts of reactants by implementation of mathematical concepts such as Calculus.

[9] Kaur, K., Jain, P., Sobti, A., & Toor, A. P. (2016). Sulfated metal oxides: eco-friendly green catalysts for esterification of nonanoic acid with methanol. *Green Processing and Synthesis*, *5*(1). https://doi.org/10.1515/gps-2015-0087

Bibliography and Literature Citation

1. Wexler, Philip. *Encyclopedia of Toxicology*. Vol. 3, Amsterdam, Academic Press, 2014, www.sciencedirect.com/referencework/9780123864550/encyclopedia-of-toxicology. Accessed 24 July 2024.
2. Chemistry LibreTexts. "Turnover Number." *Chemistry LibreTexts*, 2 Oct. 2013, chem.libretexts.org/Bookshelves/Biological_Chemistry/Supplemental_Modules_(Biological_Chemistry)/Enzymes/Enzymatic_Kinetics/Turnover_Number. Accessed 25 July 2024.
3. BYJU'S. "Esterification (Alcohol & Carboxylic Acid) - Reactions Mechanism & Uses with Videos." *BYJU'S*, 2022, byjus.com/chemistry/esterification/. Accessed 24 July 2024.
4. Liu, Yijun, et al. "Effect of Water on Sulfuric Acid Catalyzed Esterification." *Journal of Molecular Catalysis A: Chemical*, vol. 245, no. 1-2, Feb. 2006, pp. 132–140, https://doi.org/10.1016/j.molcata.2005.09.049. Accessed 30 July 2024.
5. Chemix. "Chemix - Draw Lab Diagrams. Simply." *Chemix.org*, 2019, chemix.org. Accessed 16 August. 2024.
6. Fisher Scientific. *MATERIAL SAFETY DATA SHEET Potassium Hydrogen Phthalate*. 12 Dec. 1997.
7. Bylikin, Sergey, et al. *Oxford Resources for IB DP Chemistry: Course Book*. 2023. 2023 EDITION ed., Oxford University Press, 6 Feb. 2023, Page 321. Accessed 16 August 2024

8. Master Organic Chemistry. (2014, March 6). Conversion of carboxylic acids to esters using acid and alcohols (Fischer Esterification) – Master Organic Chemistry. Retrieved from Master Organic Chemistry website: https://www.masterorganicchemistry.com/reaction-guide/conversion-of-carboxylic-acids-to-esters-using-acid-and-alcohols-fischer-esterification/
9. Kaur, K., Jain, P., Sobti, A., & Toor, A. P. (2016). Sulfated metal oxides: eco-friendly green catalysts for esterification of nonanoic acid with methanol. *Green Processing and Synthesis*, *5*(1). https://doi.org/10.1515/gps-2015-0087