Investigating the Effect of Temperature on the Buffering Capacity of an Acetate Buffer

Showmick Das[1*]

[1]International School Dhaka, Bangladesh

[1]showmickdas75@gmail.com

Advisor: Hetal Zala, hetal.zala@isdbd.org

ABSTRACT

The buffering capacity of solutions plays a critical role in various industries and biological systems, maintaining stability against pH changes when acids or bases are introduced. Buffers are integral to numerous applications, including cosmetics, pharmaceuticals, and physiological processes, such as the carbonate-bicarbonate buffer maintaining human blood at a pH of 7.4. This study investigates the effect of temperature on the buffering capacity of an acetate buffer solution, focusing on a fixed concentration of acetic acid (0.2 mol dm^{-3}) and acetate ions (0.2 mol dm^{-3}). Considering the dynamic temperature variations in real-world applications, the research aims to answer the question: *"How does varying the temperature (30°C to 70°C) affect the buffering capacity of an acetate buffer?"* The findings from this exploration provide insights into the thermal stability and efficiency of buffers under changing environmental conditions, advancing their applications in industrial and biological contexts.

1. THEORY

Acids and Bases can be strong or weak depending on their ionization, meaning the amount of H^+ or OH^- ions they can produce after being dissolved in a solution. When a strong acid or base is added to water, it completely ionizes as almost all the molecules dissociate. Conversely, when a weak acid or base is added, it only partially ionizes as most of its molecules remain undissociated (Christoph, 1987). Acids are recognized as good donors of the H^+ ions and undergo deprotonation to form a conjugate base. Whereas bases are known as good acceptors of the H^+ ion and undergo protonation to form a conjugate acid. When added to water, acids increase the concentration of H^+ ions present, whereas bases increase the concentration of OH^- ions present (Clark, 2023). Let's consider the following dissociation reaction of acetic acid:

$$CH_3COOH_{(aq)} + H_2O_{(l)} \rightleftharpoons CH_3COO^-_{(aq)} + H_3O^+_{(aq)} \qquad \text{(Flower, Eq 1)}$$
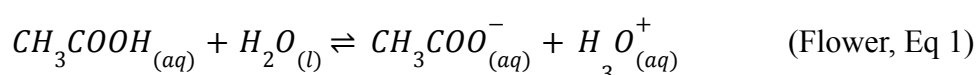
In dissociation reactions, the transfer of a proton between acids and bases results in the formation of conjugate pairs. Conjugate acid-base pairs are substances that differ by one proton. A conjugate acid is formed when the weak base accepts a proton. A conjugate base is formed when the weak acid donates a proton (Moore, 2023). In this dissociation (see equation 1), the acetic acid and acetate ion form a weak acid-conjugate base pair, whereas the water and the hydronium ion form a weak base-conjugate acid pair (Flowers, 2023). These conjugate acid and base pairs are crucial in the development of buffer solutions. A buffer comes in two types - acidic buffer and basic buffer. If a buffer is acidic, it consists of a weak acid and its conjugate base. Whereas, if a buffer is basic, it consists of a weak base and its conjugate acid. Though these are 2 different mixtures with slightly different equations, they both fulfill the same purpose. The purpose of buffers is to resist changes in pH when strong acids and bases are added to the solution. Acidic buffers are better at neutralizing the added strong bases, whereas basic buffers are better at neutralizing the added strong acids. A buffer maintains a specific pH range by neutralizing the excess hydrogen ions and hydroxide ions added to it from the strong acids and bases. For a solution to function as a buffer, the acid and base components must be part of the same equilibrium system. The dynamic equilibrium between conjugate acid-base pairs and their reversible transfer of protons is a key feature that allows them to maintain a constant pH as buffer solutions.

Let's take the example of an acetate buffer. When a strong acid is added to this buffer system, the additional H^+ ions added to the system are neutralized as they react with the base of H_2O. The reaction also forms the conjugate acid of H_3O^+. As the excess H^+ ions from the strong acid are neutralized and absorbed in the formation of H_3O^+, the pH of the system undergoes minimal change. Similarly, when a strong base is added to the buffer system, the backward reaction takes place. The H_3O^+ now acts as the acid, neutralizing the OH^- ions from the strong base while also donating a proton to CH_3COO^- which forms CH_3COOH and H_2O. This

process neutralizes the base without any significant change in pH. Buffers work through their absorption and release of protons. When a strong acid is added, the buffer can absorb the excess protons and convert them to the weak acid. Similarly, when a strong base is added, its hydroxide ions are replaced by the H^+ ions in CH_3COOH. These processes enable buffers to effectively moderate pH (Westlab, 2023).

Buffers are always in equilibrium. Adding a strong electrolyte that contains one ion in common with the reaction system will always shift the equilibrium in the direction that reduces the concentration of the common ion. This equilibrium shift is known as the common ion effect and stems from Le Chatelier's principle which states that "if a change is imposed on a system at equilibrium, the position of the equilibrium will shift in a direction that tends to reduce that change" (Zumdahl, 2007). When strong acids are added to an acidic buffer, the additional H^+ ions move the equilibrium to the left, as some of the protons react with the acetate ion to produce acetic acid. When a strong base is added, the equilibrium shifts to the right, as the additional OH^- ions get neutralized and combine with the protons to form water (Rob, 2002).

In terms of how to make a buffer solution, it's prepared through the Henderson-Hasselbach equation.

$$pH = pK_a + log\left(\frac{[A^-]}{[HA]}\right) \qquad \text{(Flower, Eq 2)}$$

Here pH is our target pH for the buffer solution, pK_a is the dissociation constant of the weak acid,
A^- is the concentration of the conjugate base, and HA is the concentration of the weak acid. By knowing the dissociation constant and target pH, we can determine the acid-base ratio needed for our buffer solution.

The performance and effectiveness of a buffer solution are determined through its buffer capacity. The buffer capacity is defined as the amount (number of moles/grams) of strong acid or base that must be added to the volume of a buffer solution to change its pH by 1 unit. Buffer breakdown occurs at the point when all the acid and conjugate bases have been used up in neutralizing the added acid or base. After this point, the addition of acid or base rapidly changes the pH, marking the buffer's limit, and marking its capacity. The buffer capacity shows the maximum amount of protons or hydroxide ions that a buffer can absorb before its pH changes significantly (Zumdahl, 2007). I will determine the buffer capacity in my investigation, as I will measure the volume of KOH added to my buffer solution before its pH changes by 1 unit. I will measure the volume of KOH added, by subtracting the initial burette reading from the final burette reading. The volume of KOH added will be converted into moles. This will be done using the $n = cv$ (Eq 3) formula. Titration is the process commonly used to make these measurements and test the buffer capacity. The optimum buffer capacity is achieved when the pH is equal to the pK_a, and when there are equal concentrations of the

two components (Rob, 2002). Using the data from the titration, the buffer capacity is ultimately calculated using the equation:

$$\beta = \frac{(amount\ of\ strong\ acid/base\ added\ in\ moles)}{(volume\ of\ buffer\ solution\ in\ dm^3)\ (\Delta pH)} \qquad \text{(Mistry, Eq 4)}$$

Since a buffer ceases to exist by definition after a pH change of 1 unit, **equation 4** can be simplified to:

$$\beta = \frac{(amount\ of\ strong\ acid/base\ added\ in\ moles)}{(volume\ of\ buffer\ solution\ in\ dm^3)} \qquad \text{(Tamhane, Eq 5)}$$

Although buffers are very effective and useful in today's industry, several factors affect their value. Such as the ratio of $[A^-]/[HA]$, the total buffer concentration, the temperature, and the ionic strength. In my investigation, I will specifically explore how the factor of temperature affects the buffering capacity. I will do so by varying the temperature of the buffer solution across $30\ °C$, $40\ °C$, $50\ °C$, $60\ °C$ and $70\ °C$ using a water bath unit.

2. HYPOTHESIS

The relationship between temperature and buffer capacity is not universally straightforward and is dependent on the specific buffer system. However, I predict that if I increase the temperature of my buffer solution, the volume of KOH required to change its pH by one unit will decrease, and hence my buffer capacity will decrease. This is largely due to Le Chatelier's principle discussed in the background theory. Dissociation of acetic acid in water has an enthalpy change calculated to be $\Delta H = -0.4\ kJ\ mol^{-1}$ (Gary L. Miessler et al, 2013). From this we can deduce that the enthalpy change (ΔH) is negative, meaning its forward reaction is an exothermic process that releases heat, whereas the backward reaction is an endothermic process that absorbs heat.

$$ln\left(\frac{K_2}{K_1}\right) = \frac{-\Delta H}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right) \qquad \text{(Tuckerman, Eq 6)}$$

Keeping this enthalpy change (ΔH) in mind, and using Van't Hoff's equation (see equation 6), we can find a relationship between the change in temperature and the equilibrium constants (such as the dissociation constant). As the dissociation of acetic acid is an exothermic process, where $\Delta H < 0$, an increase in temperature will decrease the dissociation constant (Tuckerman, 2019). Le Chatelier's principle explains this, as when a reaction at equilibrium is subjected to a change, it will respond in a way to minimize the effect of that change. In this case, it's subjected to an increase in temperature, hence the reaction will respond by decreasing the temperature, and it will do so by absorbing heat and favoring the backward endothermic reaction. As the equilibrium shifts backward and favors the reactants, the value of the dissociation constant (K_a) will reduce.

$$\beta = 2.303\left([H^+] + [OH^-] + \frac{C_{buff} \cdot K_a \cdot [H^+]}{\left([H^+] + K_a\right)^2}\right) \qquad \text{(Borkowski, Eq 7)}$$

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Using the above Van Skyle's equation, we can further deduce that a decrease in the dissociation constant (K_a) will reduce the buffer capacity of a buffer system. Hence in my investigation, I expect the graph of buffer capacity against temperature to be linear with a negative gradient. As the exothermic dissociation reaction of acetic acid involves the production of H^+ ions, an increase in temperature will shift the equilibrium backward in favor of the reactants; this will reduce the production of the H^+ ions. As the concentration of the H^+ ions reduces, the buffer neutralizes a much lower quantity of the OH^- ions released by the strong base. Due to a reduced ability of neutralization a much lower amount of strong base is required to change the pH. As the amount of strong base is proportional to the buffer capacity (see equation 4), the buffer capacity will ultimately reduce.

3. VARIABLES

Independent Variable	I *varied the temperature of the acetate buffer and the potassium hydroxide solution* using a water bath unit. I monitored the temperature of the solutions using a thermometer. I always took the solutions out of the unit when its temperature was 5 °C more than my desired temperature. Hence, even if the temperature drops it will still be very close to my desired value. I did this to minimize the effect of the heat loss to the surroundings. I varied my solutions to different temperatures. I overall collected data from 5 different temperatures - 30 °C, 40 °C, 50 °C, 60 °C, and 70 °C - conducting three trials at each temperature. I kept this range as my water bath unit couldn't give temperatures more than 70 °C and less than 30 °C. Additionally, this range of temperatures would be the easiest to maintain given the safety concerns (temperatures near boiling point could potentially burn me) as well as the school laboratory settings.
Dependent Variable	The ***buffer capacity*** is the dependent variable which will be calculated using $\beta = \frac{(amount\ of\ strong\ acid/base\ added\ in\ moles)}{(volume\ of\ buffer\ solution\ in\ dm^3)}$ (Eq 5). This calculation will require the amount of potassium hydroxide used in changing the pH by 1 unit. The amount of moles will be calculated using the $n = cv$ (Eq 3) formula, as we will utilize the data from our titration. I will conduct the titration of a strong acid, potassium hydroxide, against my acetate buffer. In the titration, I will slowly add the potassium hydroxide solution to the acetate buffer. Before starting my titration, I will record the initial reading on my 50 mL burette, as that's where the potassium hydroxide solution will be stored. As I slowly add the potassium hydroxide to the buffer, there will be an increase in the concentration of OH^- ions. This increase in OH^- ions will ultimately alter the pH of the buffer solution. This change in pH will be closely monitored using a Vernier pH sensor. Right when the pH has changed by 1 unit, the titration will be stopped. After stopping the titration I will record my final burette reading. In order to determine the volume of KOH used, I will subtract the initial burette reading from the final burette reading. The volume I find will then be inputted into the $n = cv$ equation. Knowing that the concentration of the potassium hydroxide solution will stay constant at $0.2\ mol\ dm^{-3}$, I can input that value into the equation and determine the moles of KOH added. Along with the moles of KOH, I would have known the volume of my buffer solution. Inputting the known volume of my buffer solution, as well as my calculated moles of strong acid, will ultimately allow me to calculate my dependent variable of buffer capacity.

Controlled Variables	How was it controlled?	Impact on the Experiment
Concentration of the Buffer and the Added	I will make $0.5\ dm^3$ of $0.2\ mol\ dm^{-3}$ solutions for both the acetate buffer and the potassium hydroxide. Making these large stock solutions will allow me to	As evident in equation 7, the buffer capacity depends on the buffer's concentration. Hence,

Strong Base ($mol\ dm^{-3}$)	use the same buffer solution and potassium hydroxide solution for several trials, ensuring consistency. To make $0.5\ dm^3$ of $0.2\ mol\ dm^{-3}$ potassium hydroxide, we will dissolve 5.611 grams of potassium hydroxide pellets into 500 mL of distilled water. To make the buffer solution, we would first confirm that we want our buffer's target pH to be 4.5. Additionally, acknowledging that the pKa of acetic acid (a component of the buffer) is 4.76, we will input these values into the Henderson-Hasselbach equation (see equation 2). After inputting we can determine the ratio of acetic acid and sodium acetate (has the acetate ions) in the buffer solution. Furthermore, by knowing these ratios we can obtain the volume of acetic acid and sodium acetate required in an acetate buffer which has a pH of 4.5.	this concentration will remain constant throughout. Concentration is strongly related to the buffer capacity, as larger concentration of buffer means there are more H^+ and OH^- ions available for neutralizing the added strong acid or base. Keeping the concentrations constant throughout will make the effects of the independent variable, the temperature, more evident and will minimize fluctuations from factors which aren't the focus of my investigation.
Volume of Buffer Solution (mL)	The buffer solution will be distributed for all the trials using a measuring cylinder. Utilizing this measuring tool, I will ensure each trial uses the same volume of buffer solution. I will use my measuring cylinder to precisely collect 25 mL of buffer solution. I will pour that 25 mL into the 100 mL beaker. The 100 mL beaker will then be placed in the titration setup, where the KOH will be slowly added.	The volume of buffer solution is also a key variable in the calculation of buffer capacity (see equation 4). Using the same volume of buffer will ensure equal conditions for all the titrations and keep the amount of H^+ and OH^- ions constant.
Equal Temperature of the Buffer and Titre (°C)	Both solutions will be placed in the water bath and be simultaneously heated according to the temperature required. Both the temperatures will be monitored using 2 thermometers - one in each solution.	Having different temperatures could lead to thermal exchanges between the solutions which could alter the temperature of the buffer. This would affect its ability to resist pH change and impact its buffering capacity.
Termination of the Measurement	All the titrations will be terminated as soon as the pH changes by 1 unit. This will be ensured as I will constantly monitor the pH using the Vernier pH probe. I will use the Vernier pH probe specifically due to it's added precision and minimal uncertainty of $\pm\ 0.01$. I will install the vernier app on my phone and connect the sensor to my phone via bluetooth. The use of the vernier app will not only show me the pH at an instant. Constantly being shown the pH change will allow me to stay alert and terminate the titration at the right time.	The pH change is a key factor in the buffer capacity (see equation 4). Hence calculating for the same pH change (1 unit) for all trials will ensure consistency. It will also ensure that the volume of titre (KOH) measured is accurate. Specifically calculating for pH change of 1 unit will simplify calculations and allow us to use equation 5.
Concentration of the Buffer and the Added Strong Base ($mol\ dm^{-3}$)	I will make $0.5\ dm^3$ of $0.2\ mol\ dm^{-3}$ solutions for both the acetate buffer and the potassium hydroxide. Making these large stock solutions will allow me to use the same buffer solution and potassium hydroxide solution for several trials, ensuring consistency. To make $0.5\ dm^3$ of $0.2\ mol\ dm^{-3}$ potassium hydroxide, we will dissolve 5.611 grams of potassium hydroxide pellets into 500 mL of distilled water. To make the buffer solution, we would first confirm that we want our buffer's target pH to be 4.5. Additionally, acknowledging that the	As evident in equation 7, the buffer capacity depends on the buffer's concentration. Hence, this concentration will remain constant throughout. Concentration is strongly related to the buffer capacity, as larger concentration of buffer means there are more H^+ and OH^- ions available for neutralizing the added strong acid or base.

	pKa of acetic acid (a component of the buffer) is 4.76, we will input these values into the Henderson-Hasselbach equation (see equation 2). After inputting we can determine the ratio of acetic acid and sodium acetate (has the acetate ions) in the buffer solution. Furthermore, by knowing these ratios we can obtain the volume of acetic acid and sodium acetate required in an acetate buffer which has a pH of 4.5.	Keeping the concentrations constant throughout will make the effects of the independent variable, the temperature, more evident and will minimize fluctuations from factors which aren't the focus of my investigation.

<center>Table 1: Table of Independent, Dependent and Controlled Variables</center>

4.1 APPARATUS

- $1\ dm^3\ of\ 0.2\ mol\ dm^{-3}\ Acetic\ Acid\ Solution$ (made from Acetic Acid Glacial 99 - 100%)
- $0.5\ dm^3\ of\ 0.2\ mol\ dm^{-3}\ Potassium\ Hydroxide\ Solution$ (made from Potassium Hydroxide Pellets)
- $0.5\ dm^3\ of\ 0.2\ mol\ dm^{-3}\ Sodium\ Acetate\ Solution$ (made from Sodium Acetate Cryst. Pure)
- Distilled Water
- Weighing Scale ($\pm\ 0.01$ g)
- 500 mL Volumetric Flask ($\pm\ 0.5$ mL)
- Two 250 mL Beakers ($\pm\ 0.02$ mL)
- Two 500 mL Beaker ($\pm\ 0.02$ mL)
- 100 mL Beaker ($\pm\ 0.02$ mL)
- Water Bath
- Thermometer ($\pm\ 0.5$ °C)
- Retort Stand
- Filter Funnel
- 50 mL Burette ($\pm\ 0.1$ mL)
- 50 mL Measuring Cylinder ($\pm\ 0.1$ mL)
- 100 mL Beaker ($\pm\ 0.02$ mL)
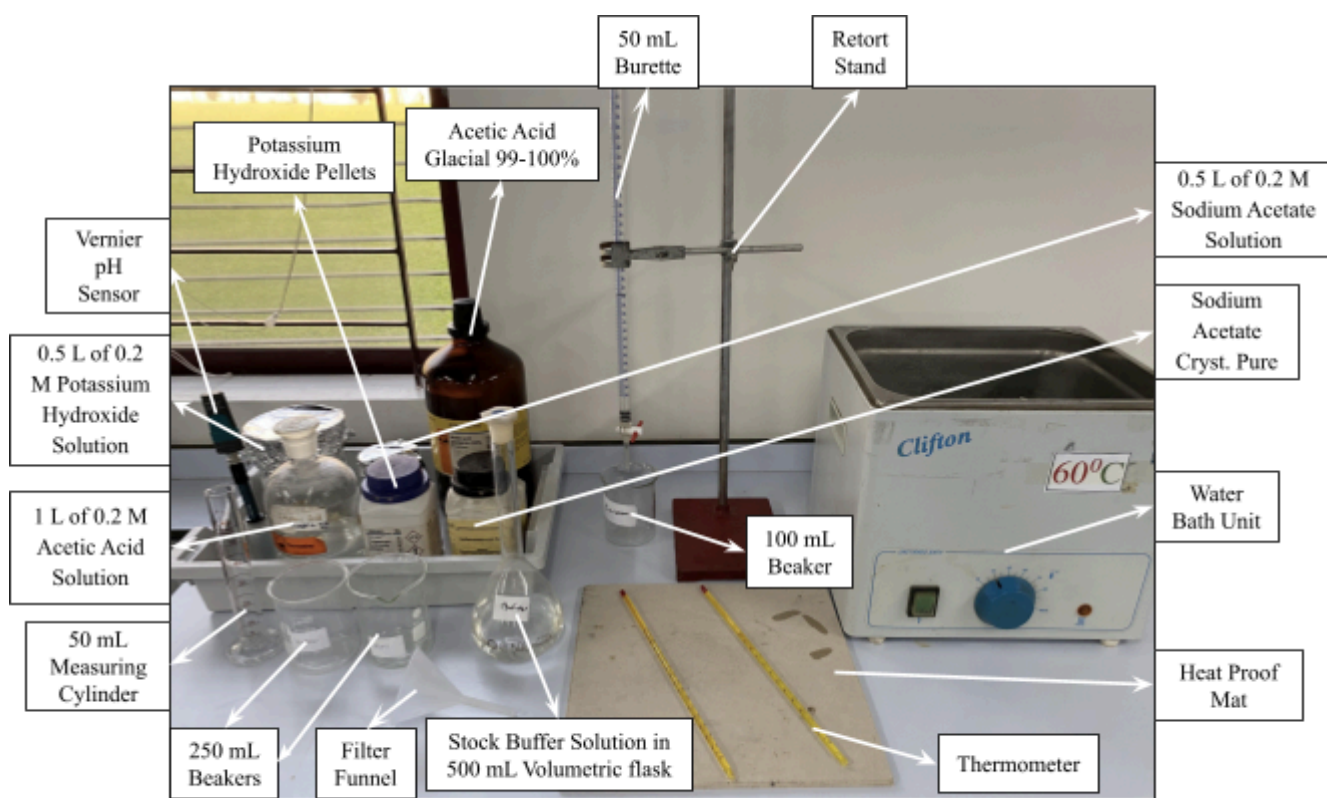- Stirring Rod
- Vernier pH Sensor ($\pm\ 0.01$)

Figure 1: Experimental Setup

4.2 METHODOLOGY

Preparing the Buffer

1. Accurately measure 2.3184 grams of sodium acetate using the weighing scale.
2. Pour the sodium acetate into a 500 mL beaker and add distilled water, diluting it to 87.5 mL. Stir until the sodium acetate has fully dissolved, giving us a $0.2 \ mol \ dm^{-3}$ solution of sodium acetate
3. Now use a measuring cylinder to accurately measure 1.912 mL of the acetic acid glacial 99 - 100%
4. Pour the 1.912 mL of acetic acid into a 500 mL beaker and add distilled water, diluting it to 162.5 mL. Stir for complete dissolution, giving us a $0.2 \ mol \ dm^{-3}$ solution of acetic acid.
5. Pour the $0.2 \ mol \ dm^{-3}$ acetic acid solution and $0.2 \ mol \ dm^{-3}$ sodium acetate solution into a 500 mL volumetric flask and stir.
6. Connect the Vernier pH Sensor to your phone and check the pH. Keep adding water to the solution and adjusting the pH until it has reached an aspired value of 4.5. This is your stock buffer solution.

Testing the performance of the Buffer solution through Titration Process

1. Pour your stock buffer solution and potassium hydroxide (strong base) into two 250 mL beakers.

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2. Prepare your water bath and place the 2 beakers inside. Monitor the temperature of each solution using a thermometer until it reaches 30 °C.
3. Once both solutions have reached 30 °C, use a filter funnel and quickly pour the potassium hydroxide into a 50 mL burette. Then, extract 25 mL of your buffer solution using a 50 mL measuring cylinder and pour it into the 100 mL beaker.
4. Record the initial pH of the buffer solution using the Vernier pH sensor and then start your titration.
5. As the titrant of KOH is slowly added, stir the buffer solution and monitor the pH change. Keep adding the titrant until the pH of the buffer changes by 1 unit.
6. Once the pH has changed by 1 unit, immediately stop the titration and record the volume of KOH used. Find this volume by subtracting the initial burette reading from the final burette reading.
7. Clean all the materials and repeat these steps 2-7 two more times at 30 °C.
8. Once done with a total of 3 trials. Repeat steps 1-7 but with temperatures of 30 °C, 40 °C, 50 °C, 60 °C and 70 °C. Record all your findings in your raw data table and use it to calculate the buffer capacity.

4.3 ETHICAL CONSIDERATIONS

As the potassium hydroxide and acetate buffer is highly caustic, contact with the skin or eyes could result in severe irritation and eye damage. Hence appropriate lab safety attire - lab coats, safety goggles, gloves - should be worn at all times. Keeping the chemical properties in mind, make sure to not drink any of the solutions throughout the experiment. Make sure all glassware and solutions are handled with care. Additionally utilize paper towels and forceps when working with solutions of higher temperatures. It should be noted that both solutions can lower the pH of waterways and be harmful to aquatic life. Hence, to be safe, at the end of each trial, allow all the solutions to cool off and be diluted with excess water before disposing them in the sink. Additionally, as I will be doing a total of 15 trials, my water bath unit will consume a lot of electricity. To minimize this wastage, I will ensure that the water bath unit is immediately turned off when not in use.

5.1 RAW DATA TABLE

Temperature of the Buffer Solution, T (°C) ± 0.5	Volume of KOH added to the Buffer Solution to increase pH by 1 unit, V/cm^3								
	Trial 1			Trial 2			Trial 3		
	Initial pH, ± 0.01	Initial Burette Reading, ± 0.05	Final Burette Reading, ± 0.05	Initial pH, ± 0.01	Initial Burette Reading, ± 0.05	Final Burette Reading, ± 0.05	Initial pH, ± 0.01	Initial Burette Reading, ± 0.05	Final Burette Reading, ± 0.05
30	4.48	0	8.2	4.44	0	8.3	4.45	0	8.0
40	4.54	0	7.8	4.53	0	7.8	4.56	0	7.6
50	4.60	0	7.2	4.63	0	7.3	4.62	0	7.2

Table 2: Raw data for the initial pH of the buffer and the burette readings of the KOH of different temperatures used in the titration

5.2 QUALITATIVE DATA TABLE

Observations	
Before Heating	Both the buffer solution and the potassium hydroxide solution are fairly transparent and have some thickness.
While Heating the Solutions	As the temperature increased, the solutions started to foam and became thinner. This is because the viscosity of the solutions reduces with an increase in temperature. Viscosity refers to the resistance of a fluid to flow. Increasing temperature generally increases the average kinetic energy of the molecules. The increased kinetic energy leads to weaker intermolecular forces, which in turn reduce a solution's viscosity. This reduction in viscosity makes a solution less resistant to flow and overall reduces its thickness. Additionally, the solutions were also seen evaporating and releasing vapor. There was also an increase in foaming and turbidity as the solutions were seen bubbling. Furthermore, the solutions also showed an increase in their degree of cloudiness and haziness as the temperature increased.
During Titration	When the potassium hydroxide solution was added to the acetate buffer, its color did not change. However, the buffer solution did become more transparent and less thick. This is largely due to the dilution which comes with the added volume of the potassium hydroxide.

Table 3: Data Table describing the Qualitative Observations

Calculating Buffer Capacity

Volume of the Buffer used for all trials = $25 \pm 0.05 \ cm^3 = 25 \pm 0.2\% \ cm^3$

Calculating for the 30 °C data point,
Volume of Potassium Hydroxide used = Final Burette Reading - Initial Burette Reading
Trial 1 = $8.20 \ cm^3$ - $0.0 \ cm^3$ = $8.20 \ cm^3$
Trial 2 = $8.30 \ cm^3$ - $0.0 \ cm^3$ = $8.30 \ cm^3$
Trial 2 = $8.00 \ cm^3$ - $0.0 \ cm^3$ = $8.00 \ cm^3$

Statistical Uncertainty,
$$\Delta n = \frac{n_{max} - n_{min}}{2} = \frac{8.30 - 8.00}{2} = 0.15 \ cm^3$$

The average volume of KOH used across all 3 trials for 10 °C,
$$V_{avg} = \frac{V_1 + V_2 + V_3}{3} = \frac{8.20 + 8.30 + 8.00}{3} = \frac{24.5}{3} \approx 8.17 \pm 0.15 \ cm^3$$

The buffering capacity is determined by the amount of moles of KOH used,
$$n_{KOH} = V \times c$$
$$n_{KOH} = (\frac{8.17 \pm 0.15 \ cm^3}{1000}) \times 0.2 \ mol \ dm^{-3} = 0.001634 \pm 0.00003 \ mol \approx 0.001634 \pm 1.836\% \ mol$$

Hence the buffering capacity at 30 °C will be,
$$\beta = \frac{\Delta B \ (amount \ of \ strong \ acid/base \ added)}{(volume \ of \ buffer \ solution)}$$

$$\beta = \frac{0.001634 \pm 1.836\% \, mol}{(\frac{25}{1000} \pm 0.2\% \, dm^3)} = 0.06536 \pm 2.036\% \, mol \, dm^{-3} \approx 0.06536 \pm 0.00133 \, mol \, dm^{-3}$$

Table 4: Sample Calculations of Buffer Capacity and Statistical Uncertainty

5.3 PROCESSED DATA TABLE

Temperature of the Buffer Solution, T (°C) $\pm$ 0.5	Average Initial pH, $\pm$ 0.01	Average Volume of KOH to Buffer Solution to increase pH by 1 unit, $V_{avg} \, (cm^3) \pm 0.05$	Buffer Capacity	Absolute and Percentage Uncertainty
30	4.46	8.17	0.06536	$\pm$ 0.00133 (2.04%)
40	4.54	7.73	0.06184	$\pm$ 0.000924 (1.49%)
50	4.62	7.23	0.05784	$\pm$ 0.000516 (0.89%)
60	4.66	6.83	0.05464	$\pm$ 0.000509 (0.93%)
70	4.71	6.33	0.05064	$\pm$ 0.0009013 (1.78%)

Table 5: Processed data for the average volume of KOH added during the titration and the buffer capacity at different temperatures
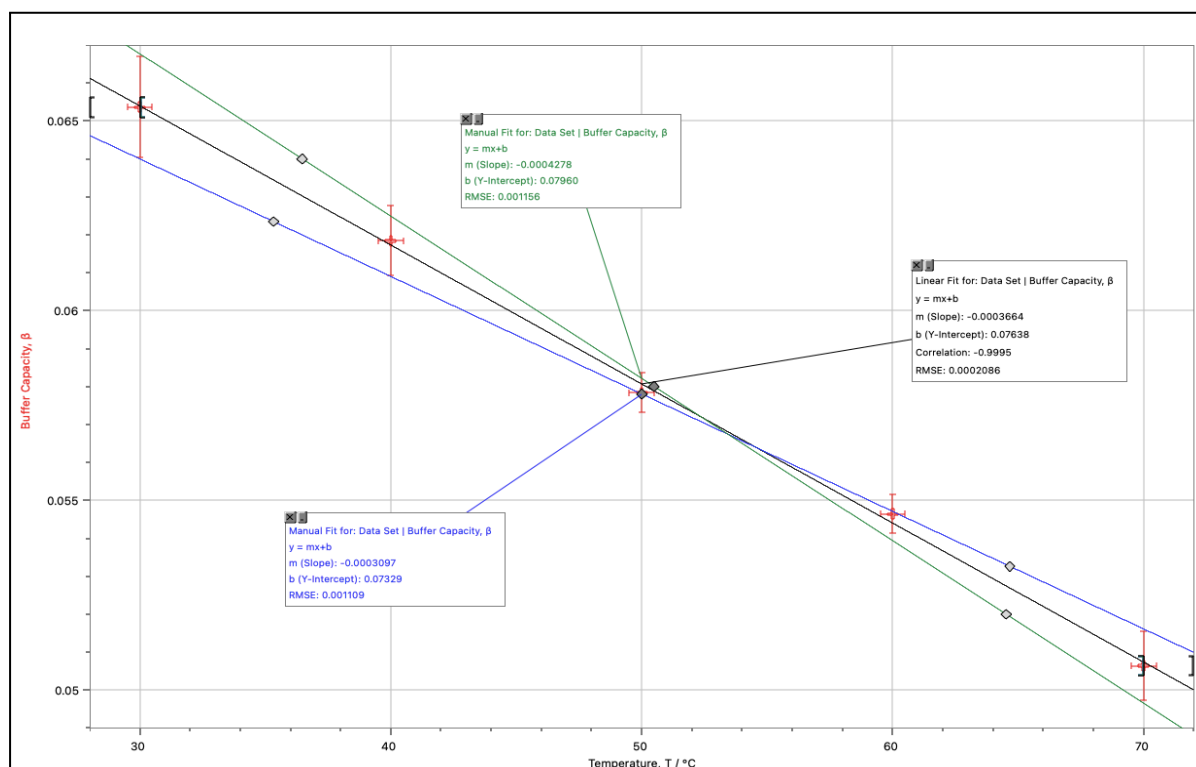
6. GRAPH

Figure 2: Graph of Buffer Capacity against Temperature

As seen in Figure 2, our graph of temperature versus buffer capacity gives us a linear relationship with the following equation: $\beta = 0.07638 - 0.0003664T$ (Eq 8) with a

minimal uncertainty of ± 0.0030959. The uncertainty was calculated by adding the slope and intercept uncertainty from equations 9 and 10: $\Delta m + \Delta b = 0.0000591 - 0.003155 = \pm 0.0030959$.

Y - Intercept Uncertainty of the Line of Best Fit	Gradient Uncertainty of the Line of Best Fit
$\Delta b = \frac{Max\ intercept - Min\ intercept}{2}$ (Eq 9) Max Line y-intercept = 0.07329 Min Line y-intercept = 0.07960 Line of Best Fit y-intercept = 0.07638 $\Delta b = \frac{0.07329 - 0.07960}{2} = \frac{-0.00631}{2}$ $\Delta b = -0.003155$ $b = 0.07638 \pm 0.003155$ $b = 0.07638 \pm 4.13\%$	$\Delta m = \frac{Max\ gradient - Min\ gradient}{2}$ (Eq 10) Max Line Gradient = -0.0003097 Min Line Gradient = -0.0004278 Line of Best Fit Gradient = -0.0003664 $\Delta m = \frac{-0.0003097 - (-0.0004278)}{2} = \frac{0.0001181}{2}$ $\Delta m = 0.0000591$ $m = -0.0003664 \pm 0.0000591$ $m = -0.0003664 \pm 16.13\%$

Table 6: Propagating Errors in the Graphical Model

7. ANALYSIS

My results and model show an inversely proportional relationship between buffer capacity and temperature. The graph's equation (see equation 8) not only supports my hypothesis but also has a minimal error with an uncertainty of ± 0.0030959. The graph gives such a low uncertainty primarily due to the error bars. The vertical error bars are moderately sized and not too large. This stemmed from the uncertainty of ± 0.05 in the burette when measuring the volume of strong base added. Additionally, as I conducted 3 trials and took their average, I not only reduced the random error but also calculated the statistical uncertainty which ranged from ± 0.05 to ± 0.15. These low values show my data's precision and tight range, aiding the low error in my buffer capacity calculations and reducing the size of my vertical error bars. On the other hand, my horizontal error bars remained constant at a value of ± 0.5. This was moderately high as we used an analog thermometer whose smallest scale division was 1 °C. Though most of the error bars were fairly standard and not too large, my first and last data points had the highest statistical uncertainties which caused the maximum and minimum lines to be further apart. Though those two points were within the line of best fit, they can be considered anomalous due to their high statistical uncertainties. But as those points were within the line of best fit, the error wasn't too extreme. However, the points did ultimately lead to a higher percentage uncertainty of 16.13% in the -0.0003664 gradient of my line of best fit. The y-intercept gave more desirable results with a value of 0.07638 and an absolute uncertainty of ± 0.003155 which aided a much lower percentage uncertainty of 4.13%.

8. CONCLUSION

In conclusion, the experiment's results indicate the validity of my hypothesis. The linear graph (see Figure 2) with a negative gradient supports my prediction that the buffer capacity will decrease as the temperature of the solution increases. With every 10 °C increase in temperature, the buffer capacity is reduced by an average of 0.003664. This is largely because when the temperature of the buffer increases the buffer deviates from its optimal conditions.

With an increase in temperature, the concentration of buffer components decreases. Additionally, the ratio of the concentration between the weak acid and conjugate base also deviates from the optimal ratio of 1 (Mistry, 2021). This is largely due to the equilibrium shifts which change the concentrations of the reactants and products. Using Le Chatelier's principle, we say that the temperature increase in exothermic reactions causes it to favor the backward endothermic reaction in an attempt to minimize the effect of the added temperature. As the reaction shifts backward towards the reactants, there's a decrease in the dissociation constant as well as the production of the H^+ ions. As the concentration of H^+ ions decrease, the buffer's pH increases, becoming a weaker acid. As the pH increases, the buffer again deviates from its optimal point. The optimal point is when the pH of the buffer is equal to the pKa of the weak acid, which in our case is the acetic acid with a pKa of 4.76 (Tamhane, 2021). As there is a minimized production of H^+ ions, the buffer neutralizes a much lower quantity of OH^- ions from the strong base. Due to a reduced ability of neutralization, the buffer capacity ultimately reduces, as a much lower volume of strong base is required to change the pH. Van Skyle's equation (see equation 7) also supports this, as the concentration of H^+ ions are proportional to the buffering capacity. Meaning, as the concentration of H^+ ions reduce, the buffering capacity also reduces (Borkowski, 2022). As we previously stated, the optimal buffering capacity is dependent on the concentration of H^+ and OH^- ions available. As the increase in temperature shifts the equilibrium to the left, it causes a reduction in the production of these ions which ultimately reduces the amount of strong acid or base it can neutralize, thus reducing its buffering capacity. As buffer capacity depends on the concentrations of the buffer components it is a very dynamic property that is very case-specific. Thus there are no literature values for me to compare with. However, my results can still be verified as my graphical model only had an uncertainty of ±0.0030959 and my calculations of buffer capacity had low percentage uncertainties of 0.89% to 2.04%. Additionally, my model is also capable of interpolating and extrapolating, as it can make accurate predictions regarding the buffer capacity even 37 °C out of the known range. This was confirmed using online buffer capacity calculators.

9. EVALUATION

When reflecting upon my experiment, I identified a couple of strengths. Without a doubt, this experiment is centered around buffer capacity. Hence, the percentage uncertainties in the calculation of buffer capacity ranging in low values of 0.89% to 2.04% is a testament to the effectiveness of my method. I had a strong range of testing values, as I worked with 5 different data points, changing the temperature from 30 °C to 70 °C. This range is strong, especially considering the school lab conditions. Even though more data points are possible, working with temperatures near the freezing and boiling point would lead to more errors and safety concerns. As I managed to conduct 3 trials at each data point, this allowed me to take an average and reduce my random error, while also giving me sufficient data to create an accurate graphical model that can interpolate and extrapolate for a larger range of values. These strong numerical values ultimately aid the small error bars on my graph, visually representing the accuracy of my investigation. My trials were a lengthy process as I

constantly reheated the solutions in order to minimize the temperature fluctuations. Hence, conducting the titration right next to the water bath unit made this a significantly smoother process. A key reason why I had a sufficient amount of data is that I had effectively planned out my experiment and made large stock solutions: more than 500 mL of acetate buffer and potassium hydroxide solution. This gave me plenty of volume to work with and even allowed me to conduct some trial runs. The practice from the trial runs ultimately reduced my random human error, and the lack of extreme outliers is evidence of that. I also took other experimental measures as I made sure to rinse all my beakers and the pH probe after every trial. Additionally, taking the temperature to more than 5 °C of the required temperature and conducting the titration as fast as possible next to the water bath unit also allowed me to reduce the heat loss to the surroundings. Similarly, simultaneously heating the two solutions and carefully monitoring them allowed me to minimize any thermal exchanges that could fluctuate the buffer's temperature.

Type of Error	Influence on Experiment	Improvement
Systematic Error	The **heat loss to surroundings** was the most major error in my experiment. This error was most prominent when working with higher temperatures. I constantly reheated and rushed the titration to keep the effect of the temperature, but this ultimately only led to more errors in determining the volume of KOH used in changing the pH. This further reduced the accuracy of the buffer capacity calculations. These limitations ended up giving my graph large error bars when working with higher temperatures. This reduced the accuracy of my experiment, giving the gradient of my linear model a high uncertainty of 16.13%.	The heat loss to surroundings can be minimized next time by carrying out the titration in an insulated heat chamber. Taking place in a more isolated system would minimize the heat escaping and how much the solution is influenced by surrounding temperatures. Additionally, next time it would be effective to heat up the individual equipment such as the pH probe, as that would prevent the thermal exchange between the solution and the equipment.
Random Error	**Fluctuations in the Vernier pH probe** at times gave me unstable values for the initial pH. This led to random error which was evident in my first and last trials which had the highest statistical uncertainty ultimately leading to large vertical error bars at those data points. These large error bars caused errors in my gradient and y-intercept, giving it a high percentage of errors. This overall reduced the accuracy of my model and caused it to face limitations in its ability to extrapolate.	Next time I can further utilize the large stock solutions by conducting more trial runs at the start of the experiment. This would allow me to test out the pH probe and other equipment for errors. In case I notice errors I can keep multiple pH probes at my disposal. This would allow me to minimize error and not use fluctuating probes. Additionally, taking 3 to 5 measurements of the initial pH and taking the average would reduce the random error, overall enhancing my accuracy.
Random Error	Though I had utilized my stock solutions to conduct some practice runs, my experiment still encountered **human error**. This was especially prominent in the higher temperatures, as at times I was unable to stop the titration on time. This led to inaccuracies regarding the volume of KOH used to change the pH. This human error caused some large error bars, which ultimately reduced the accuracy, giving the gradient a high uncertainty.	Next time I can implement the use of video analysis for identifying the exact moment when the pH changes by 1 unit, as well as the exact volume of the burette at that moment. Such frame-by-frame analysis will significantly reduce random human error, leading to a more accurate graphical model. Additionally, the usage

		of digital burettes can also reduce error and lead to more preciseness regarding the exact volume of the burette during 1 pH change.
Systematic Error	I faced **measurement and instrument errors** as my apparatus had fairly high uncertainties due to most of it being analog equipment. My measurement of the volume of KOH utilized analogue equipment such as a burette which gave an uncertainty of ± 0.05 cm³. Additionally, using an analog thermometer gave an uncertainty of ± 0.5 °C. This influenced my results leading to the value of the y-intercept as well as the 4.13% percentage uncertainty in it.	In order to achieve higher precision, digital equipment could be used next time. Using a digital burette and digital thermometer would reduce the uncertainty in my measurement tools. Additionally, measuring the values 3 to 5 times and taking an average will further reduce the possible random error in these measurements, and improve my precision and reliability.

Table 7: Evaluating the experiment's limitations

10. FURTHER INQUIRY

In order to enhance my knowledge of buffers it would be intriguing to compare the buffer capacities of monoprotic weak acid buffers, diprotic weak acid buffers, and triprotic weak acid buffers; The diprotic and triprotic weak acid buffers having more than one buffer region would allow for more complex explorations. As this investigation explored the effects of temperature on buffer capacity, it could be extended to explore the effects of concentration. Additionally, as this experiment utilized only 5 temperature data points, it could be further extended to investigate the buffer capacity at more extreme temperatures, as that would significantly affect the dissociation constant.

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